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Modeling for nuclear data: state-of-the-art and future perspectives

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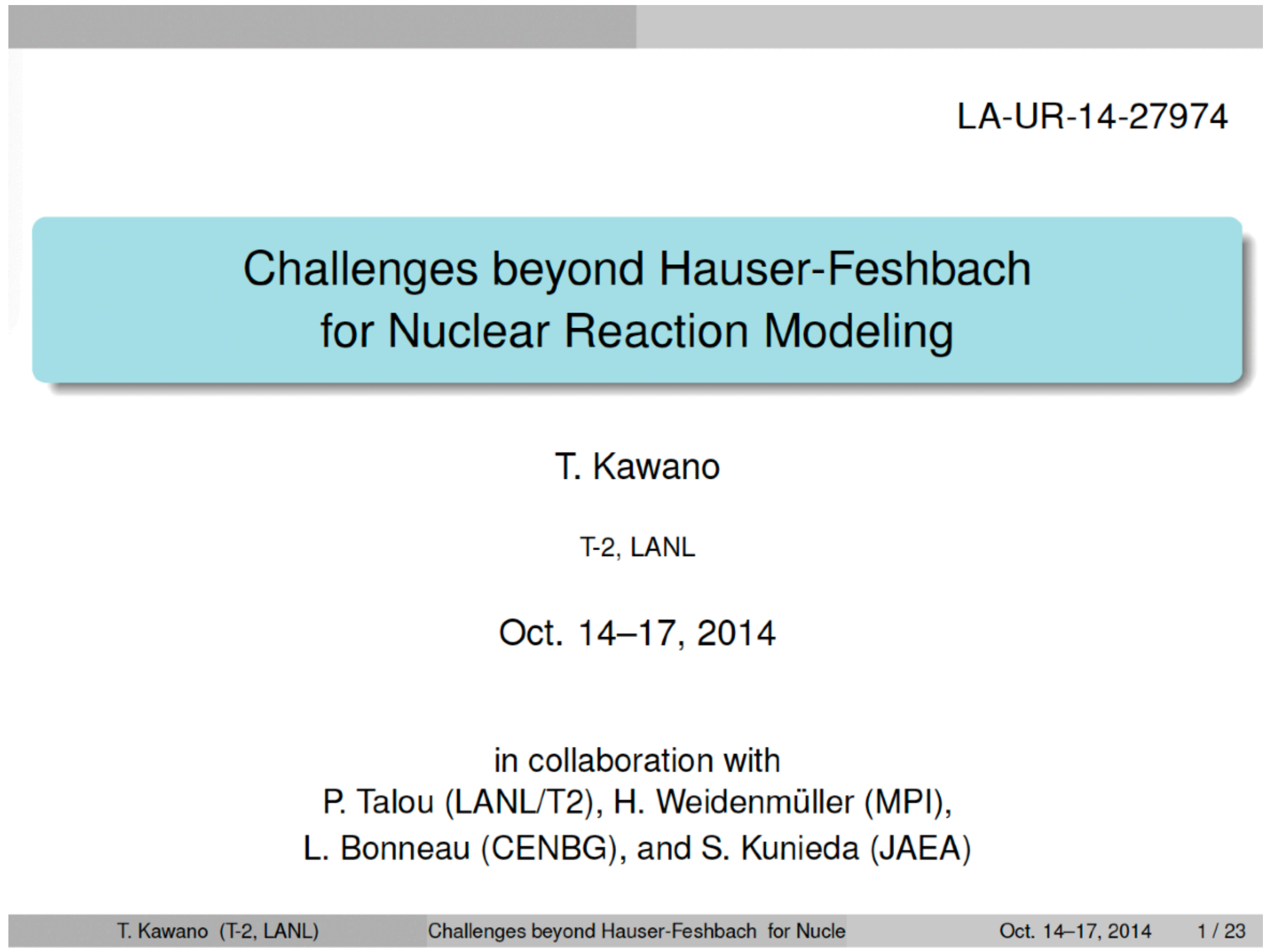
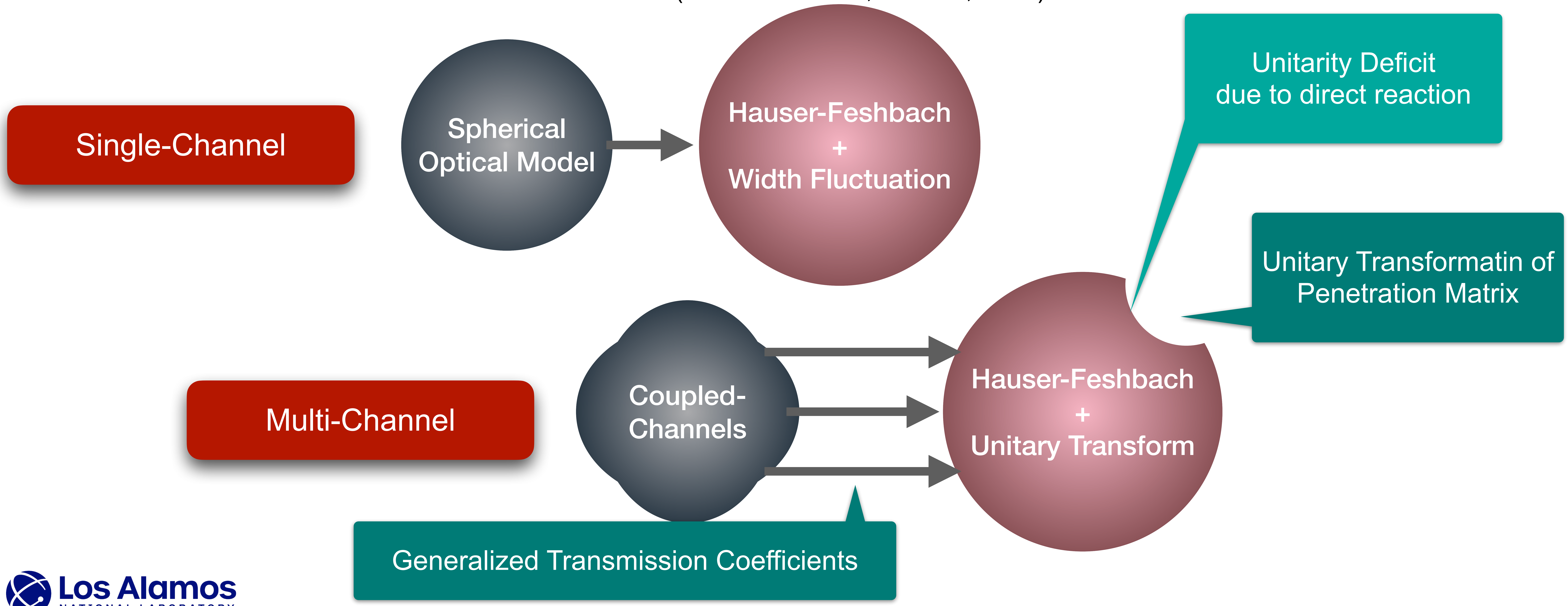
What I Told at P(ND)^2-2 in 2014

- **Challenges beyond Hauser-Feshbach for Nuclear Reaction Modeling**
  - **GOE statistics for width fluctuation**
  - **Correct treatment of direct reaction channels essential**
    - Engelbrecht-Weidenmueller transformation, or KKM
  - **Nuclear structure (mean-field calculation) input**
    - Direct/Semidirect capture with Hartree-Fock or FRDM single-particle wave functions
    - Pre-equilibrium process in terms of the microscopic particle-hole excitation
  - **Uncertainties in the photon and fission channels**
    - Photon transmission coefficient from the GDR model
    - Fission calculation still unsatisfactory
- **In the following slides I will show the recent findings**
  - which directly impacted on the nuclear data production



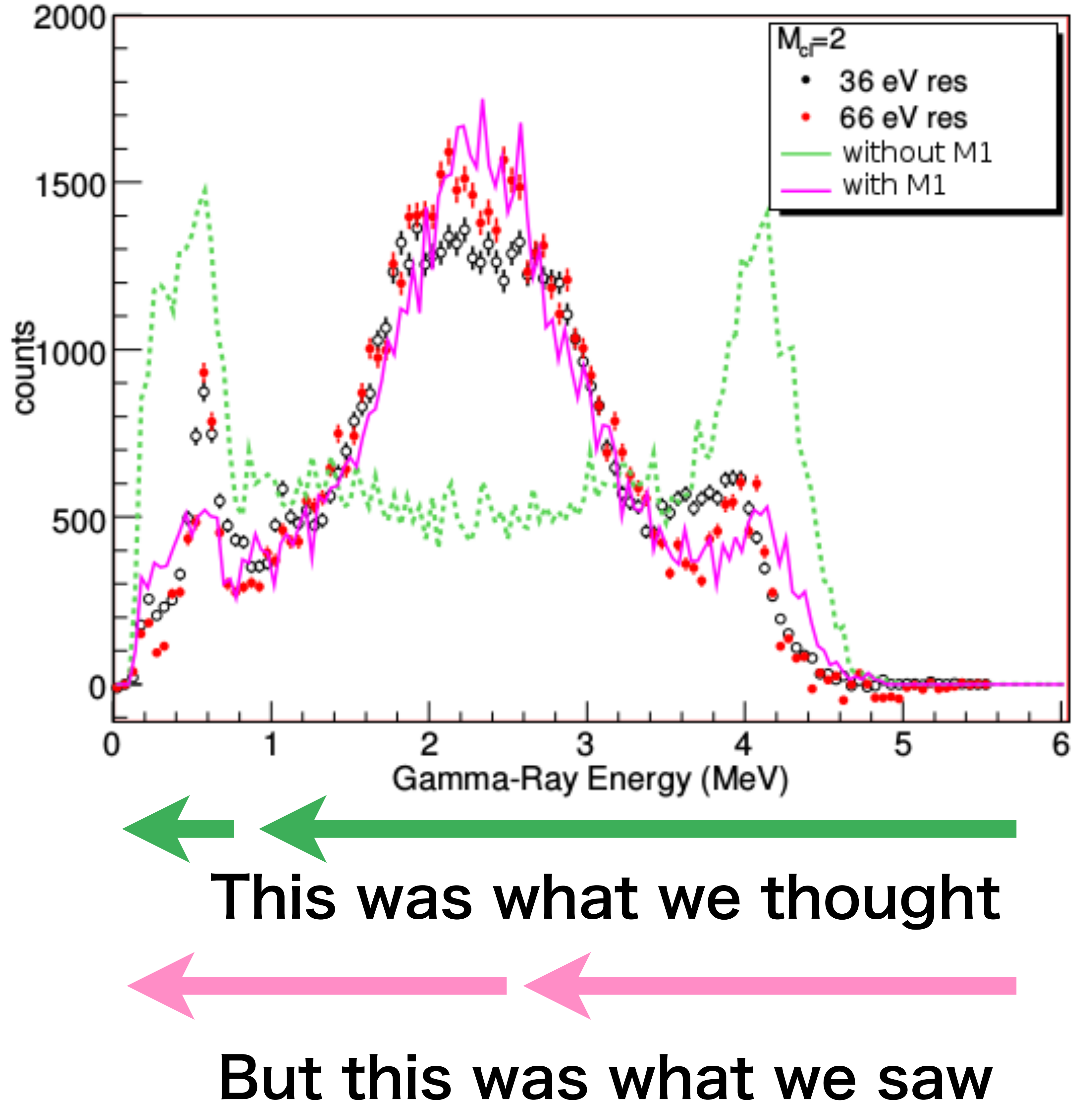
What happened during the last decade, I

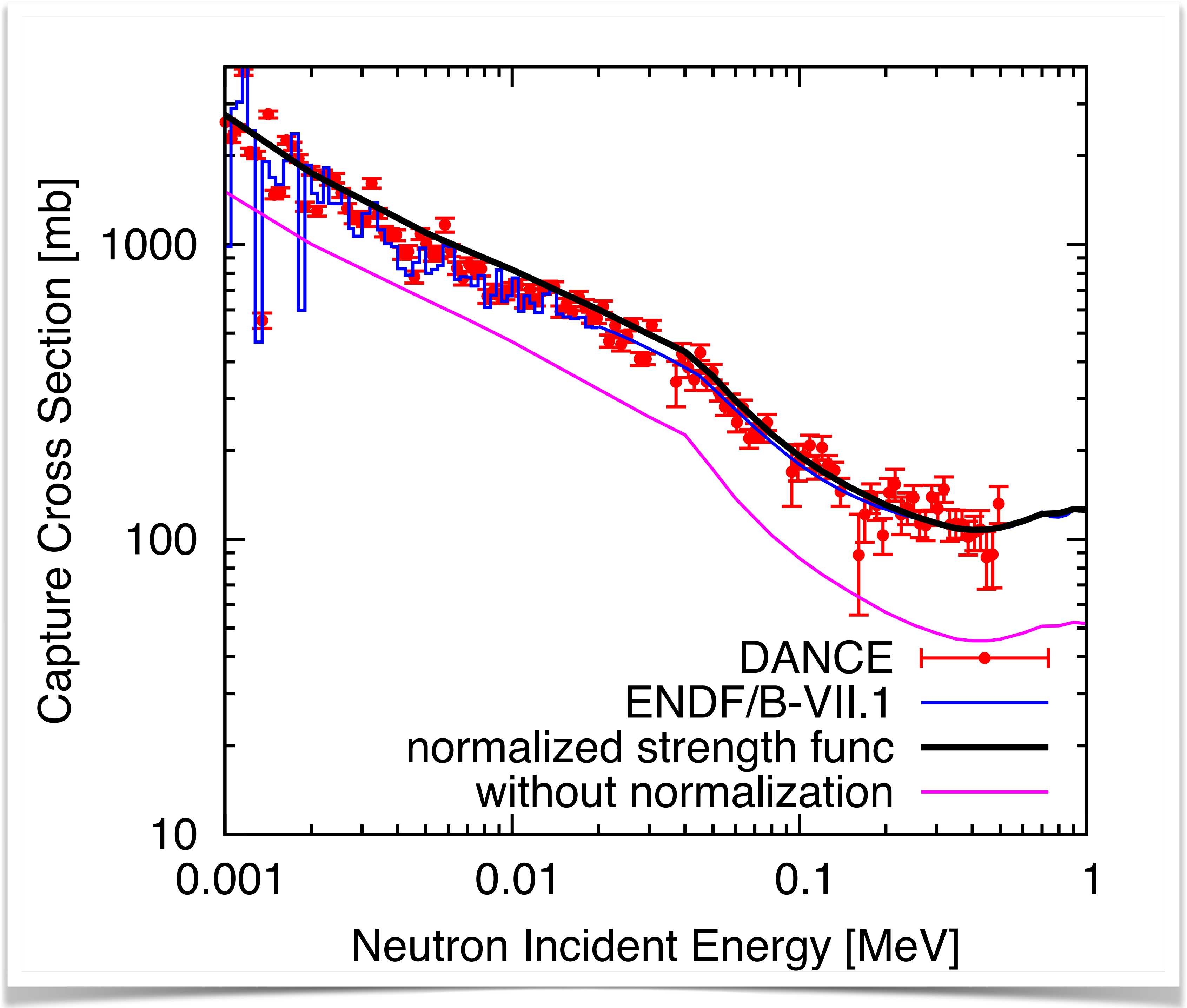
- **GOE statistics for width fluctuation, and correct treatment of directreactions**
  - New parameterization gives very accurate compound cross section (Kawano PRC92, 044617, 2015)
  - Direct reaction in the same framework (Kawano PRC94, 014612, 2016)



What Happened during the Last Decade, II

- **Gamma-ray strength function for deformed nuclei**
  - 2 step gamma-ray cascade by DANCE (Ullmann, PRC89, 034603, 2014)
  - Oslo method for Th, Pa, and U isotopes (Guttormsen, PRC89, 014302, 2014)

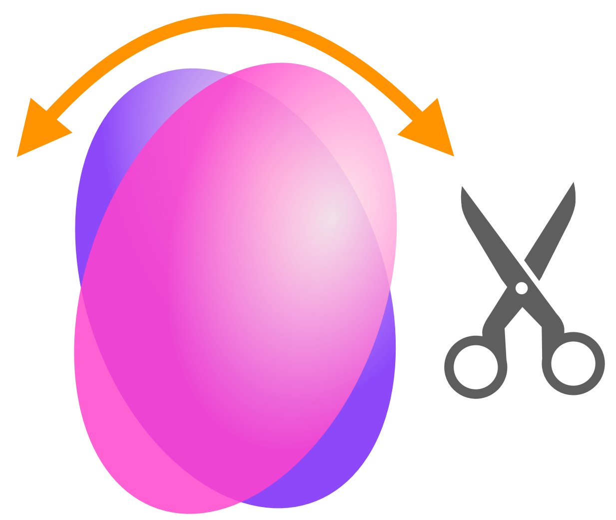




Some groups thought that this is an E1 pygmy resonance

But this was a magnetic dipole transition - Scissors mode

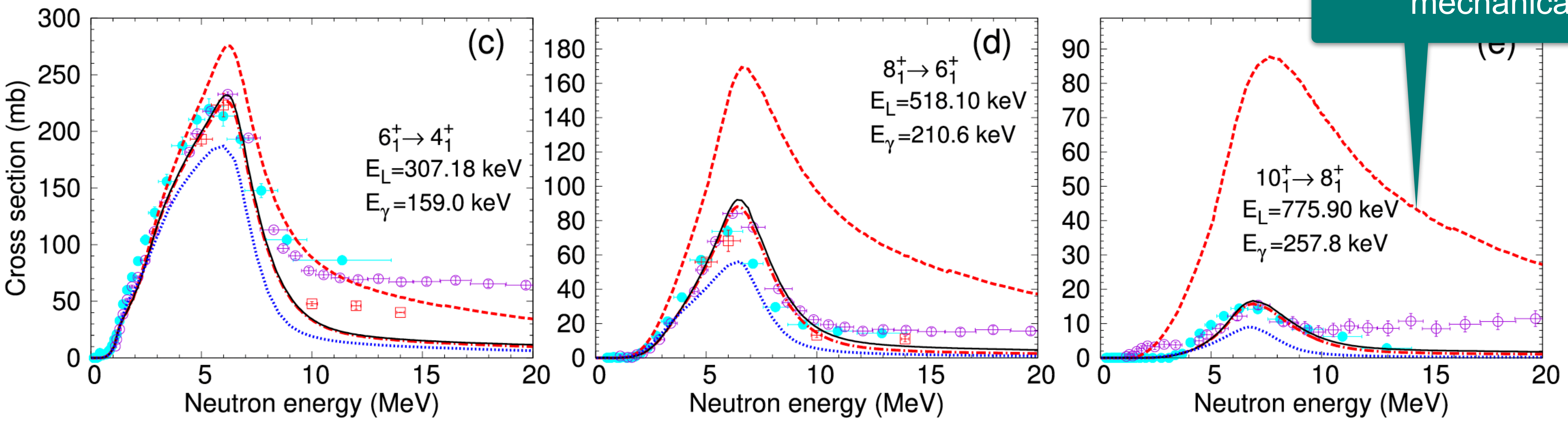
Prediction of capture cross section for deformed nuclei significantly improved



What Happened during the Last Decade, III

- **Gamma-ray production by neutron inelastic scattering off deformed nuclei**
  - ^{238}U(n,n'g) measurement at GELINA demonstrated issues in the spin-transfer during the pre-equilibrium process (Kerveno, PRC104, 044605, 2021)
  - Similar phenomena reported at LANSCE, GEANIE

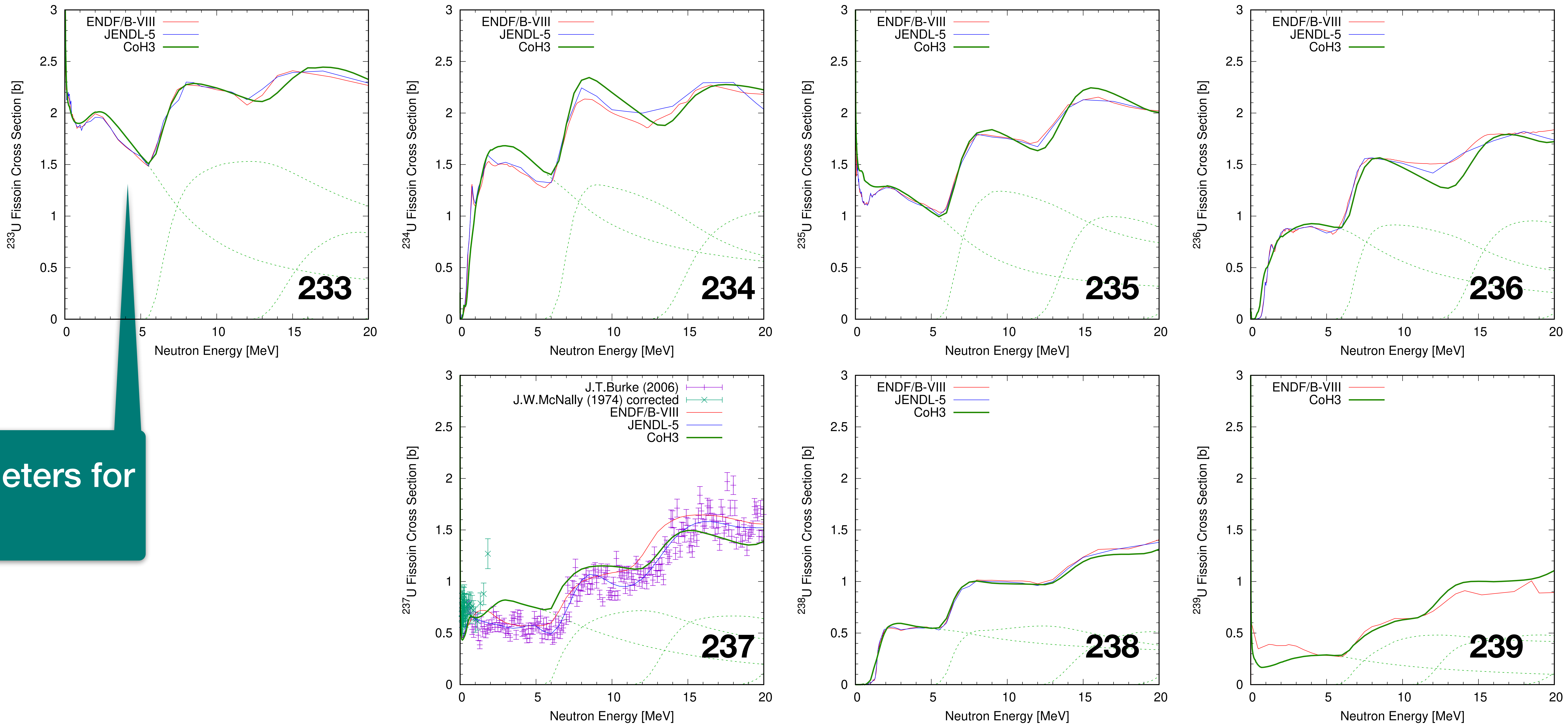
Requires to consider quatum mechanical effects



Population of higher spin states is strongly suppressed due to limited number of collisions in PE

What Happened during the Last Decade, IV

- **Fission channel in Hauser-Feshbach calculation**
  - Fission penetrability through one-dim potential (Kawano, PRC107, 044610, 2024)
  - Finally we are able to provide a unique set of fission parameters



Same fission parameters for ^{234}U used

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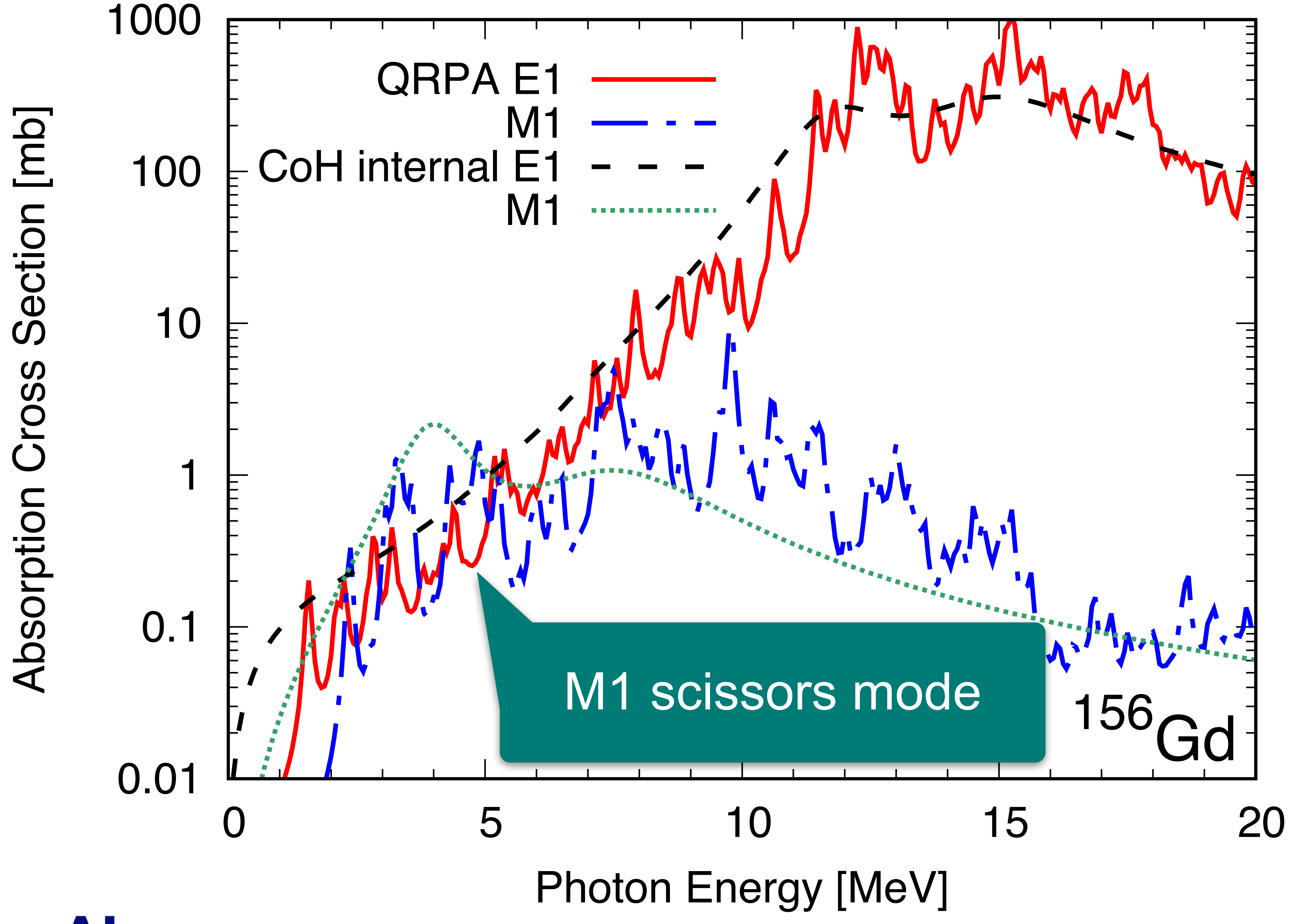
Step Forward

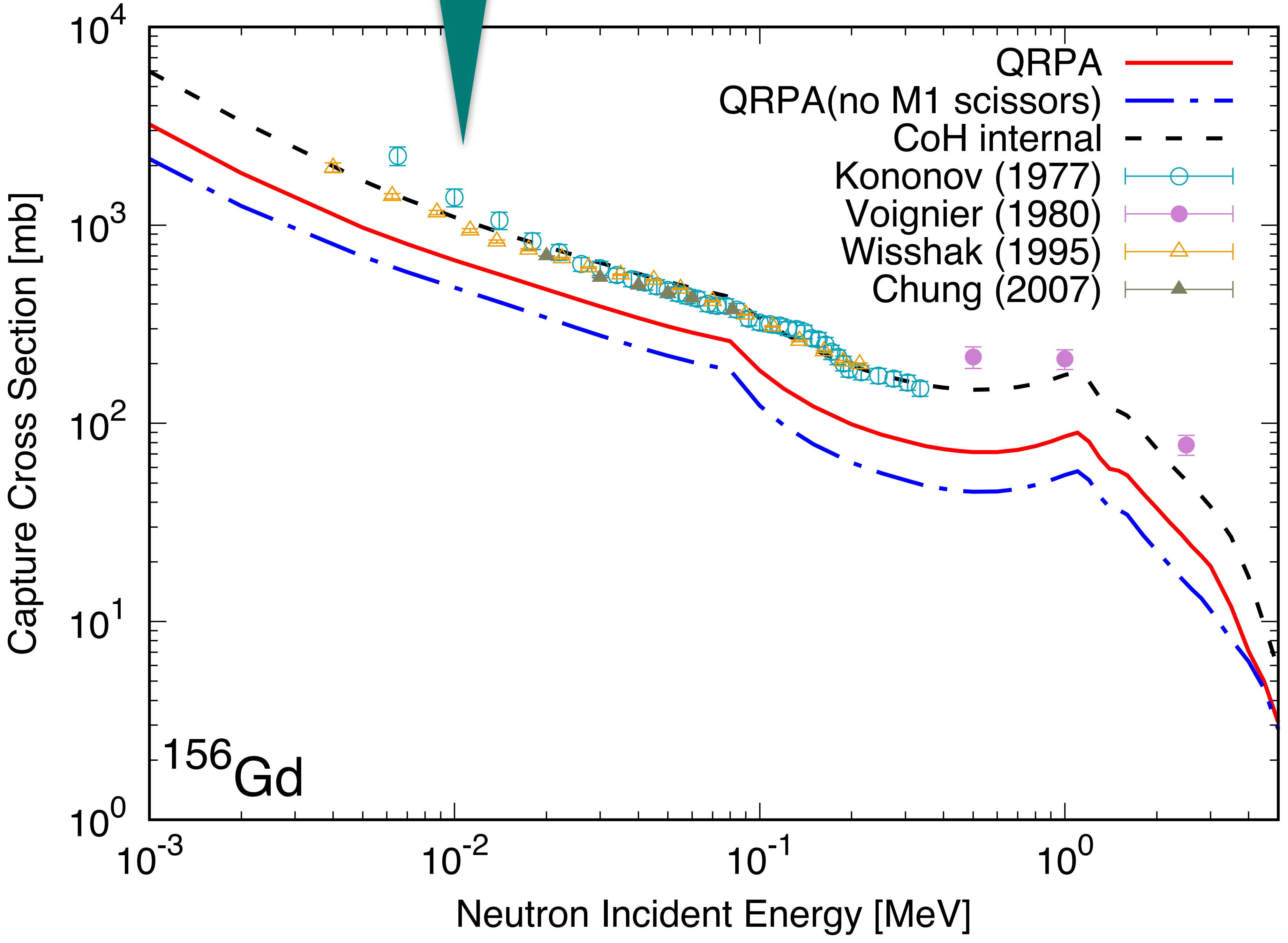
- **Things already happening, and things that may emerge in the next decade**
- **QRPA for nuclear excitation by electromagnetic interaction**
  - Photo-absorption calculation with QRPA/FAM including both E1 and M1
    - done by several groups
- **More quantum mechanical descriptions for nucleon scattering**
  - QRPA and FAM for nuclear reactions
    - direct reaction by (Q)RPA (Dupuis, PRC100, 044607, 2019)
    - direct and pre-equilibrium reactions by non-iterative FAM (Sasaki, PRC112, 054607, 2025)
- **Consistent modeling of all fission observables**
  - Fission fragment decay with the Hauser-Feshbach model
    - HF3D (Haser-Feshbach Fission Fragment Decay) model (Okumura, JNST55, 1009, 2018)
    - multi-chance fission implementation (Lovell, PRC103, 014615, 2021)
- **... and more**

Non-Iterative Finite Amplitude Method (Photons and Pre-Equilibrium)

- **Fast calculation of QRPA developed by H. Sasaki**
  - Iteration procedure not required
  - So far applied to
    - photo-absorption (gamma-ray transmission coefficient)
    - Neutron inelastic scattering



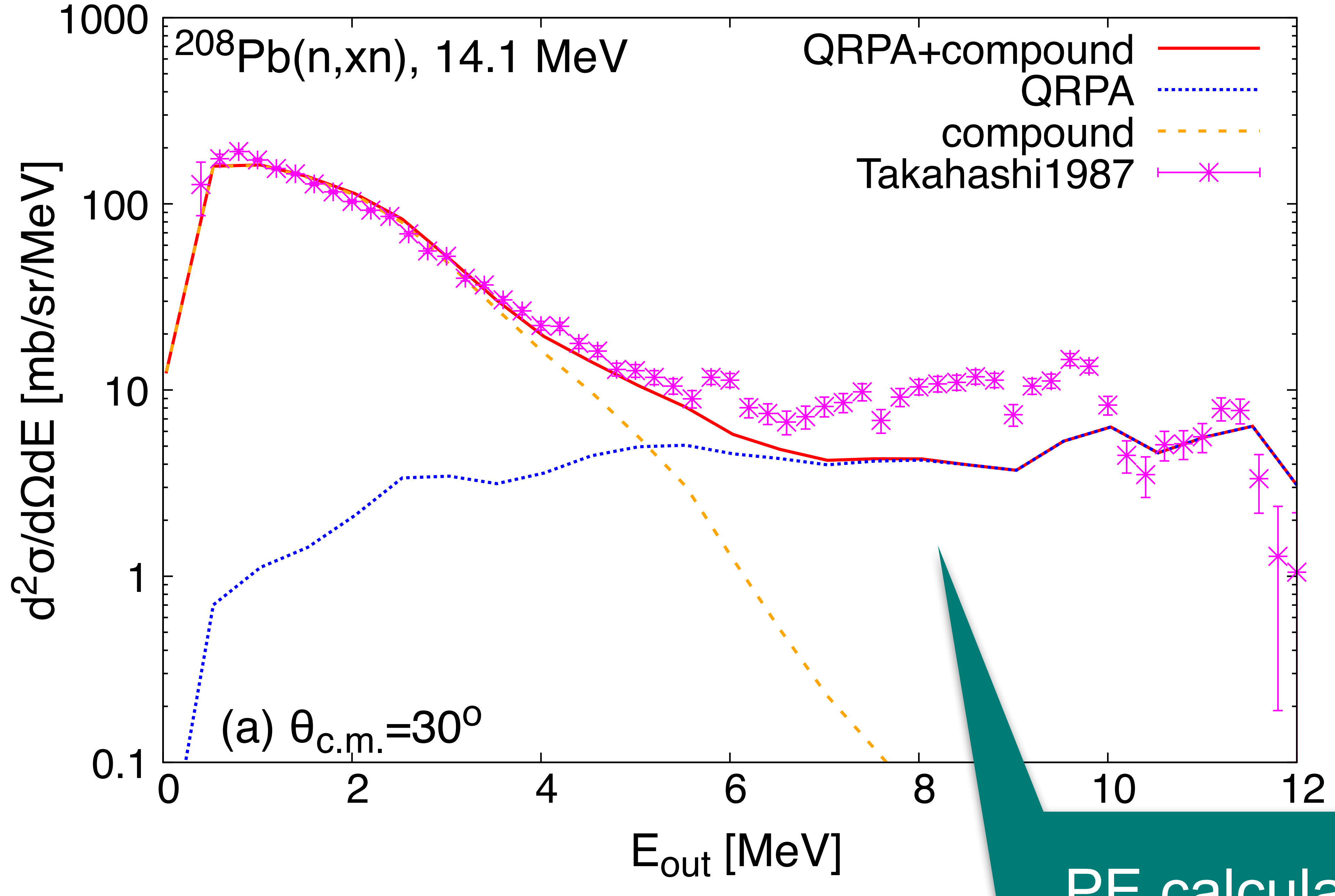
GDR parameters applied to neutron capture calculation

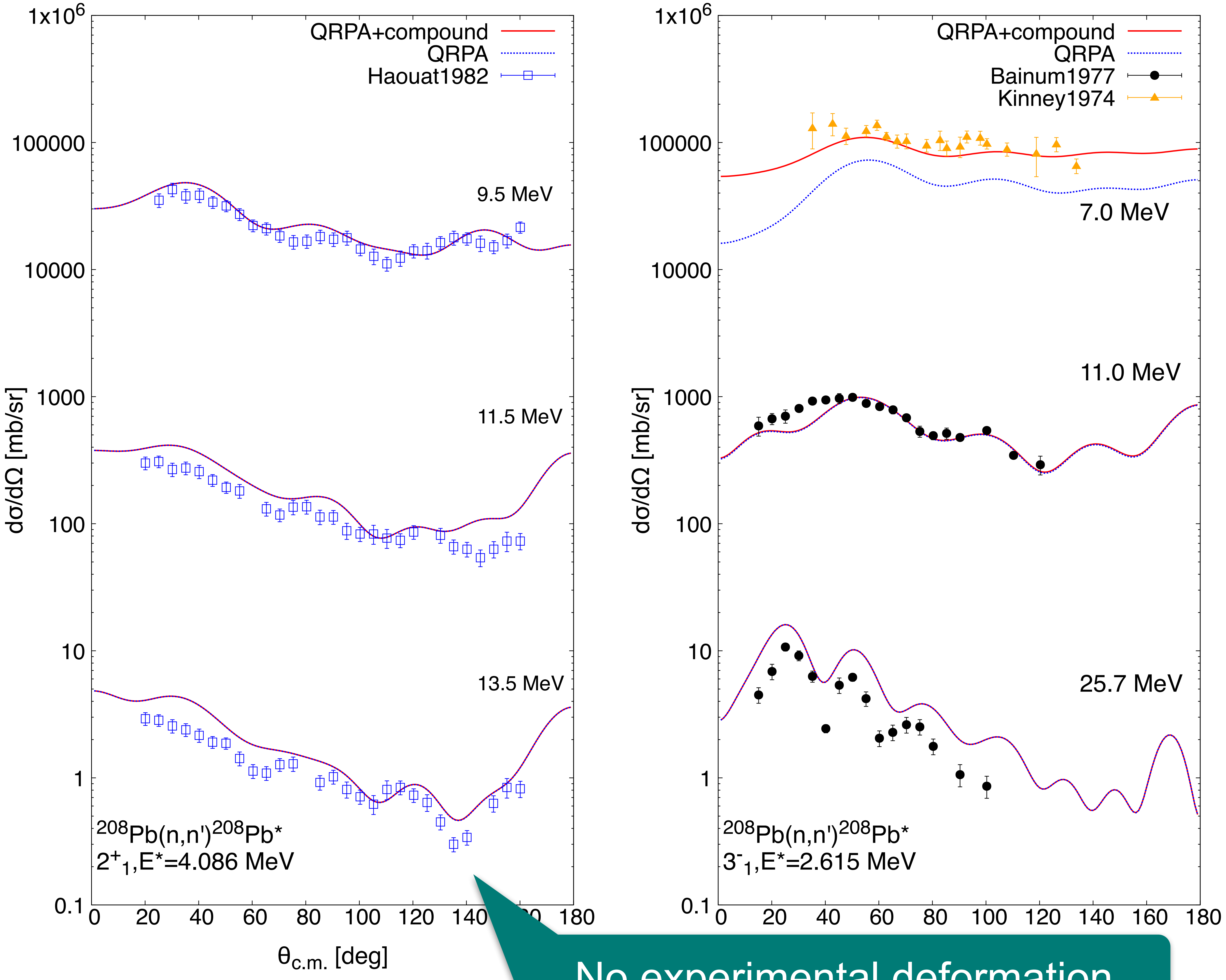


H. Sasaki, PRC107, 054312 (2023)

Inelastic Scattering off ^{208}Pb, No Adjustable Parameters

- **Microscopic approach to calculate (n,n') c.s. for both discrete and continuum final states**
  - non-Iterative FAM
  - provide realistic spin transfer to residual
  - related to gamma-ray production issues





PE calculation, same basis as DI

No experimental deformation parameters needed

H. Sasaki, PRC112, 054607 (2025)

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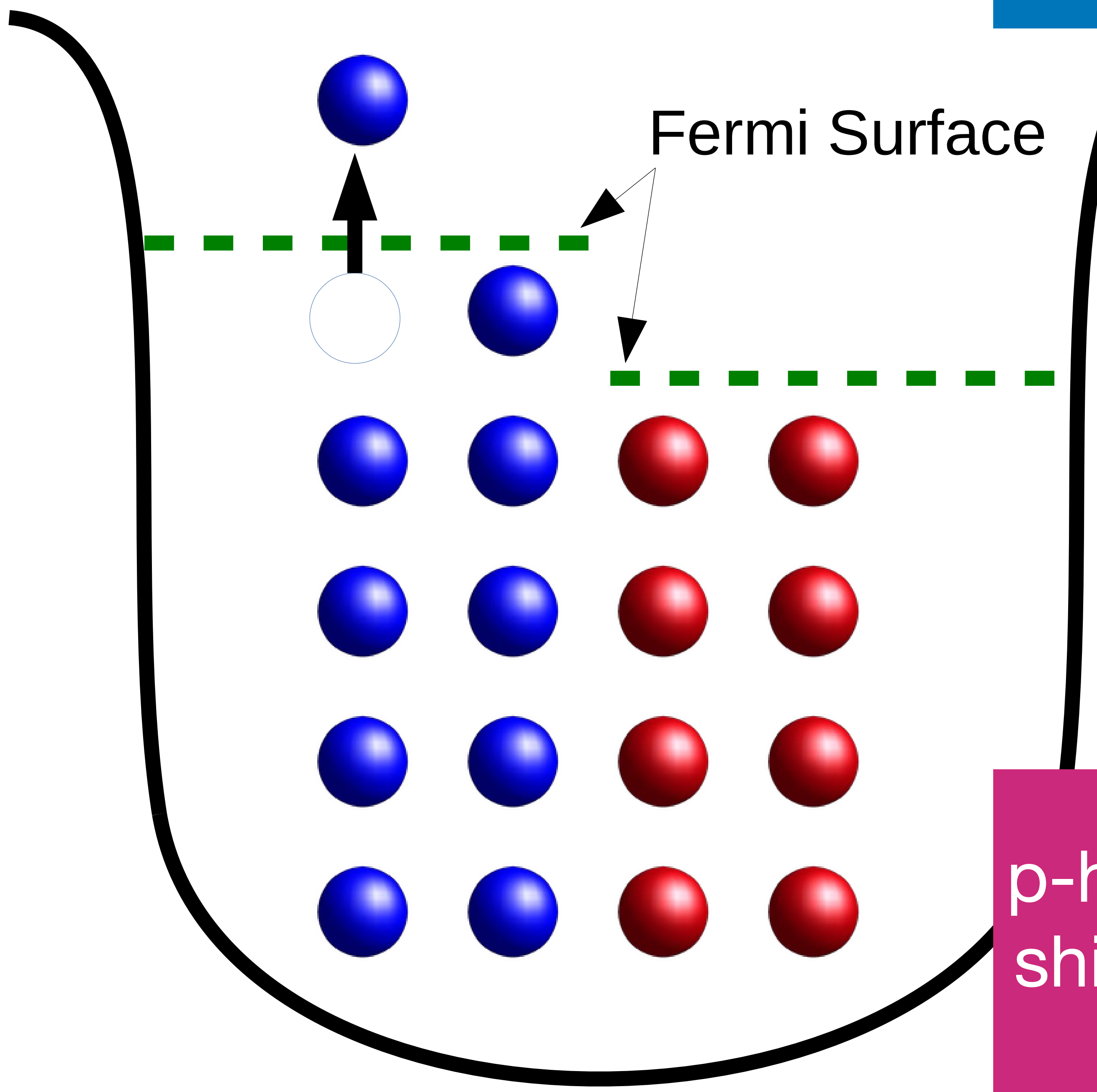
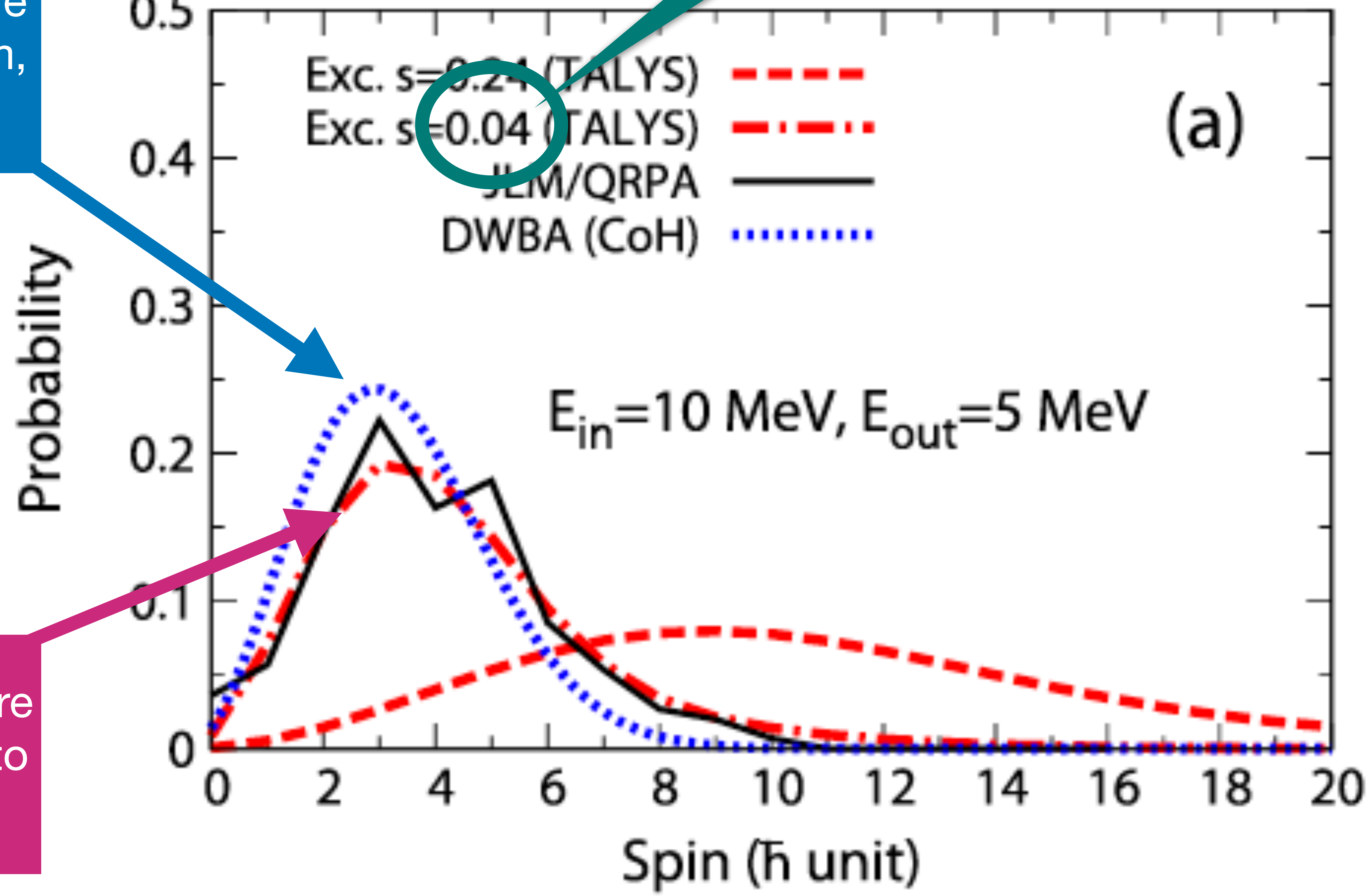
CEA and LANL Models for Spin Transfer in Pre-Equilibrium Process

Why this value is so small?

p-h configuration energies are from single-particle spectrum, no shift, no width

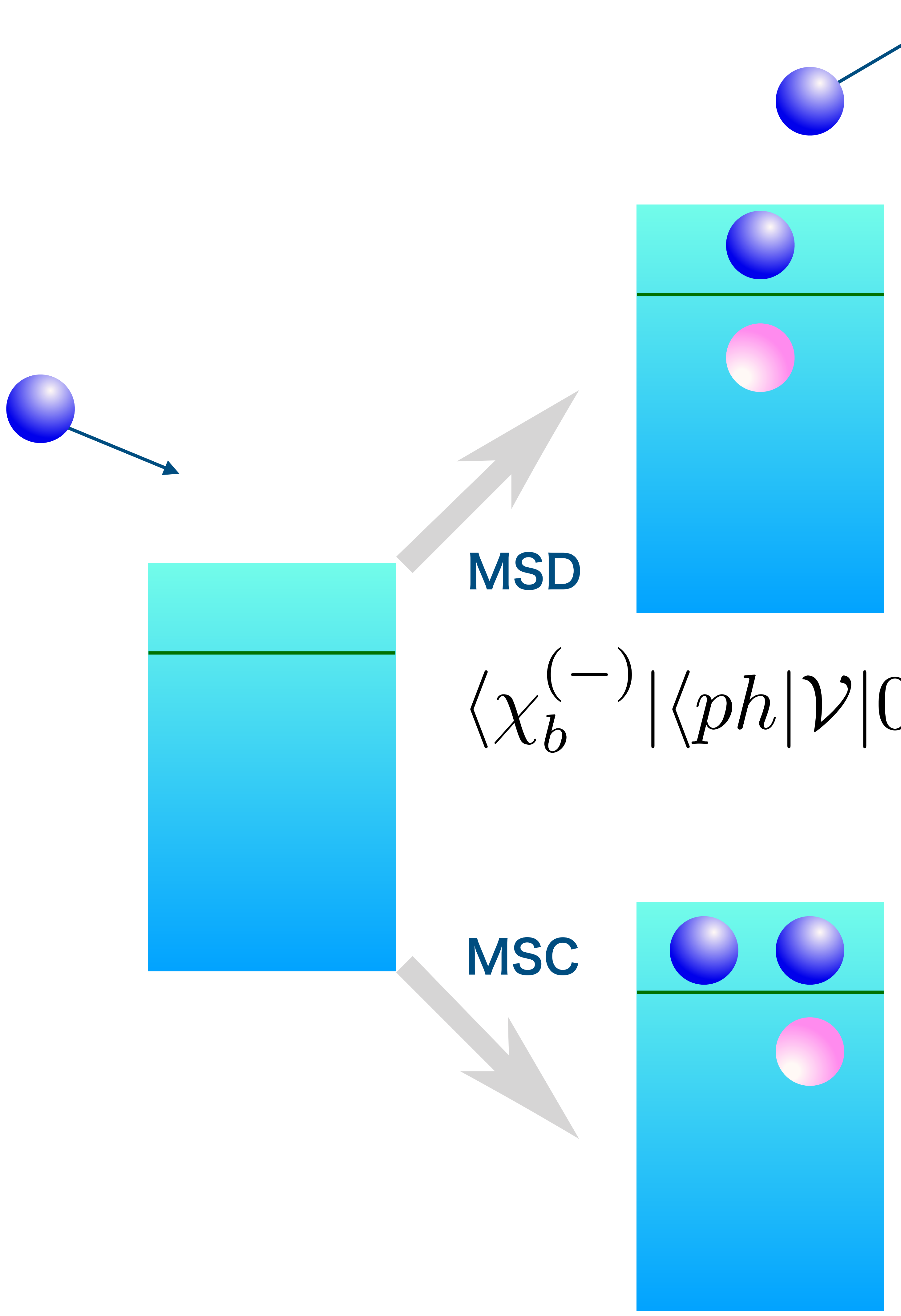


p-h configuration energies are shifted and distributed due to residual interaction



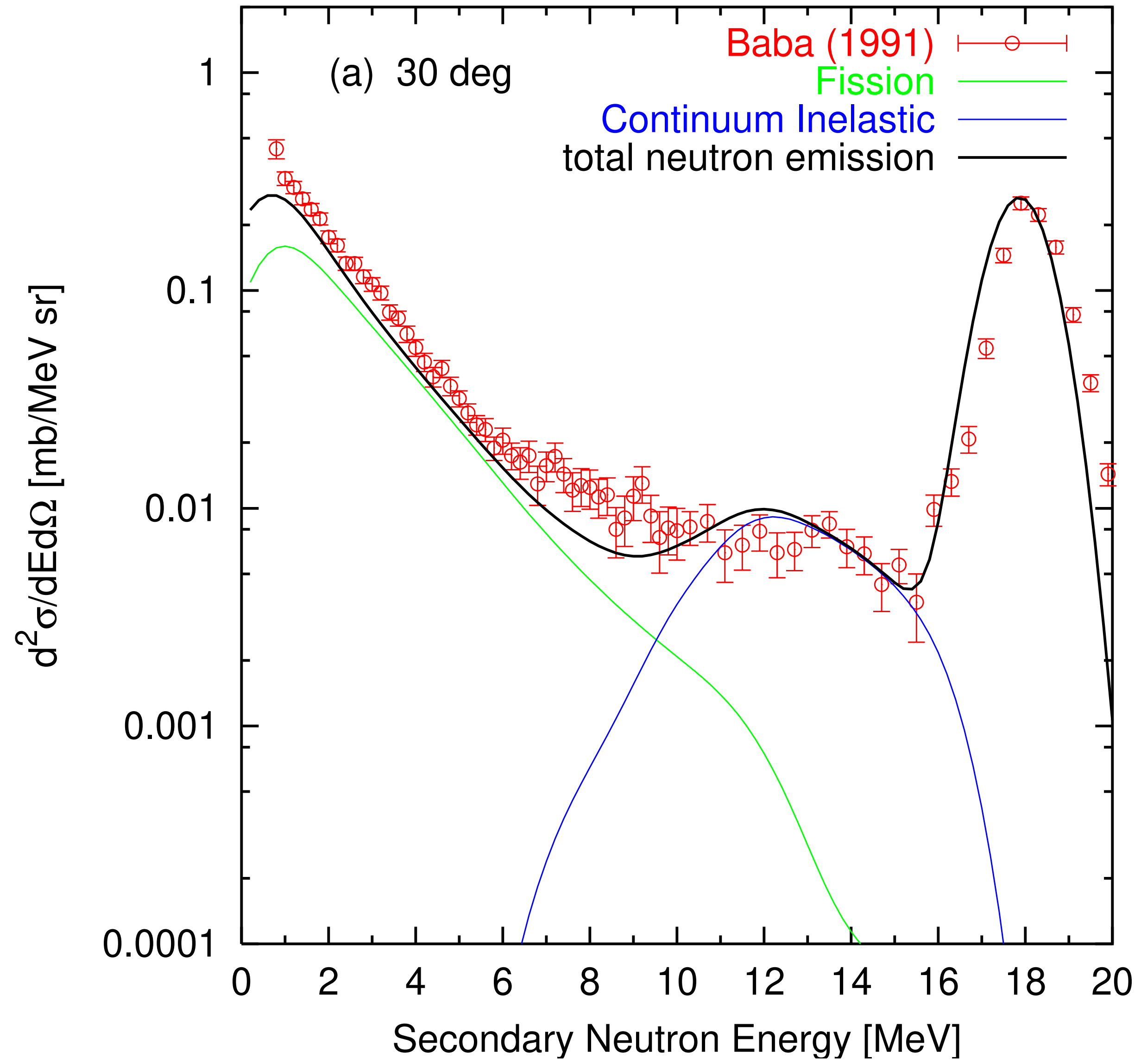
Kerveno, PRC104, 044605 (2021)

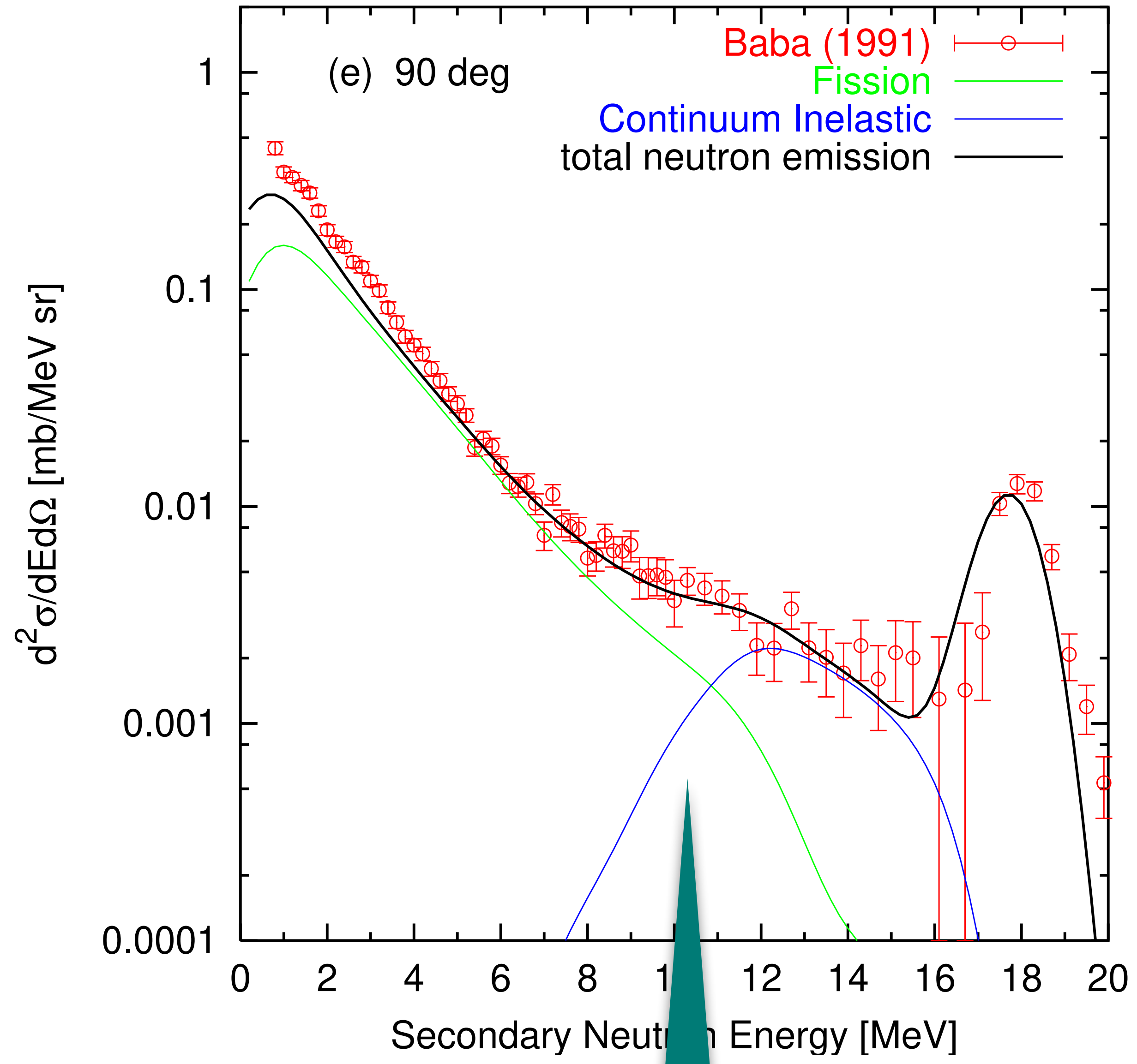
One-Step Reaction, DWBA to Continuum



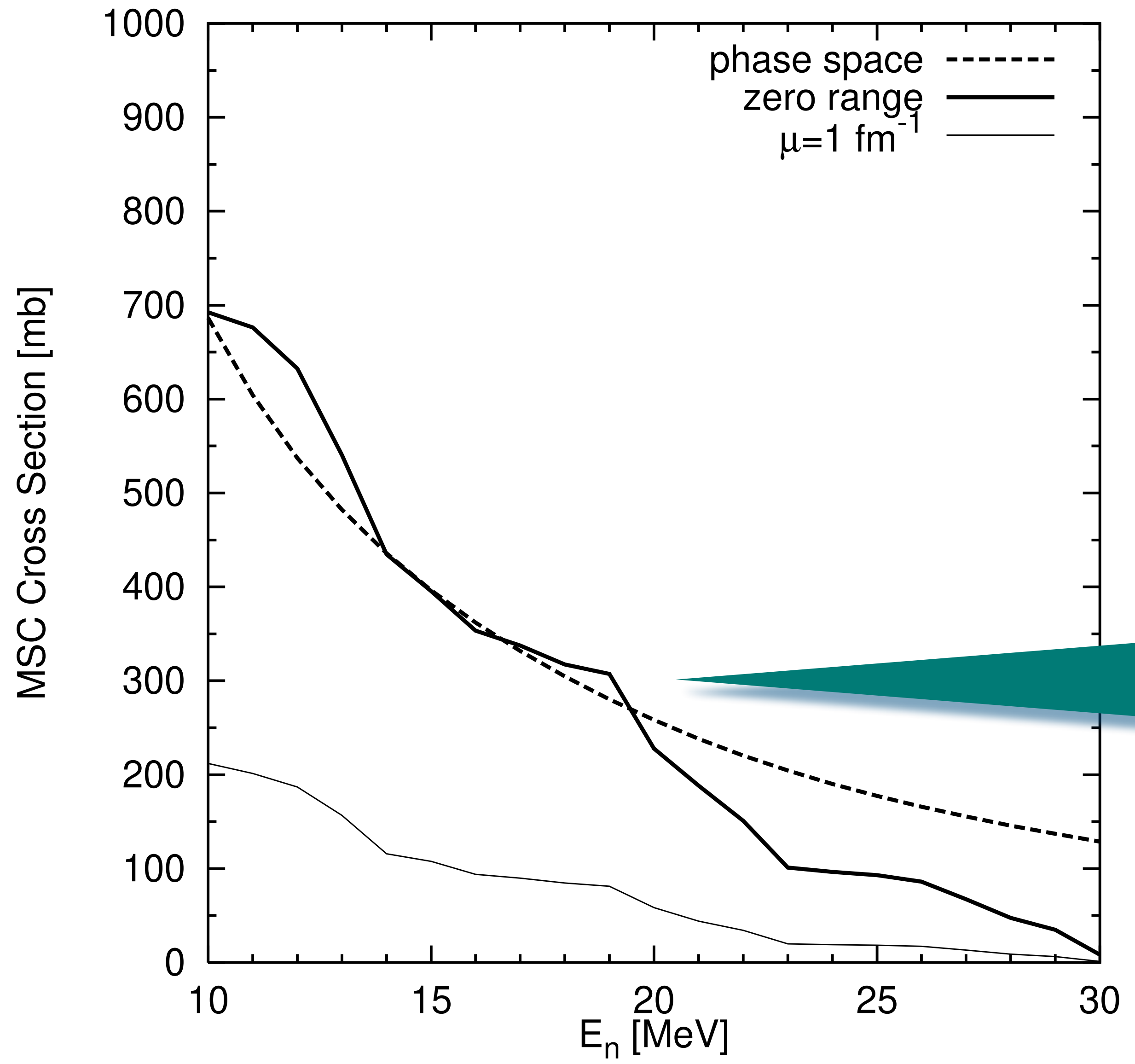
$$\langle \chi_b^{(-)} | \langle ph | \mathcal{V} | 0 \rangle | \chi_a^{(+)} \rangle$$

$$\langle u_b | \langle ph | \mathcal{V} | 0 \rangle | \chi_a^{(+)} \rangle$$





One-step process reproduce experimental data resonably



Entrance formation probability decreases as the incident energy increases

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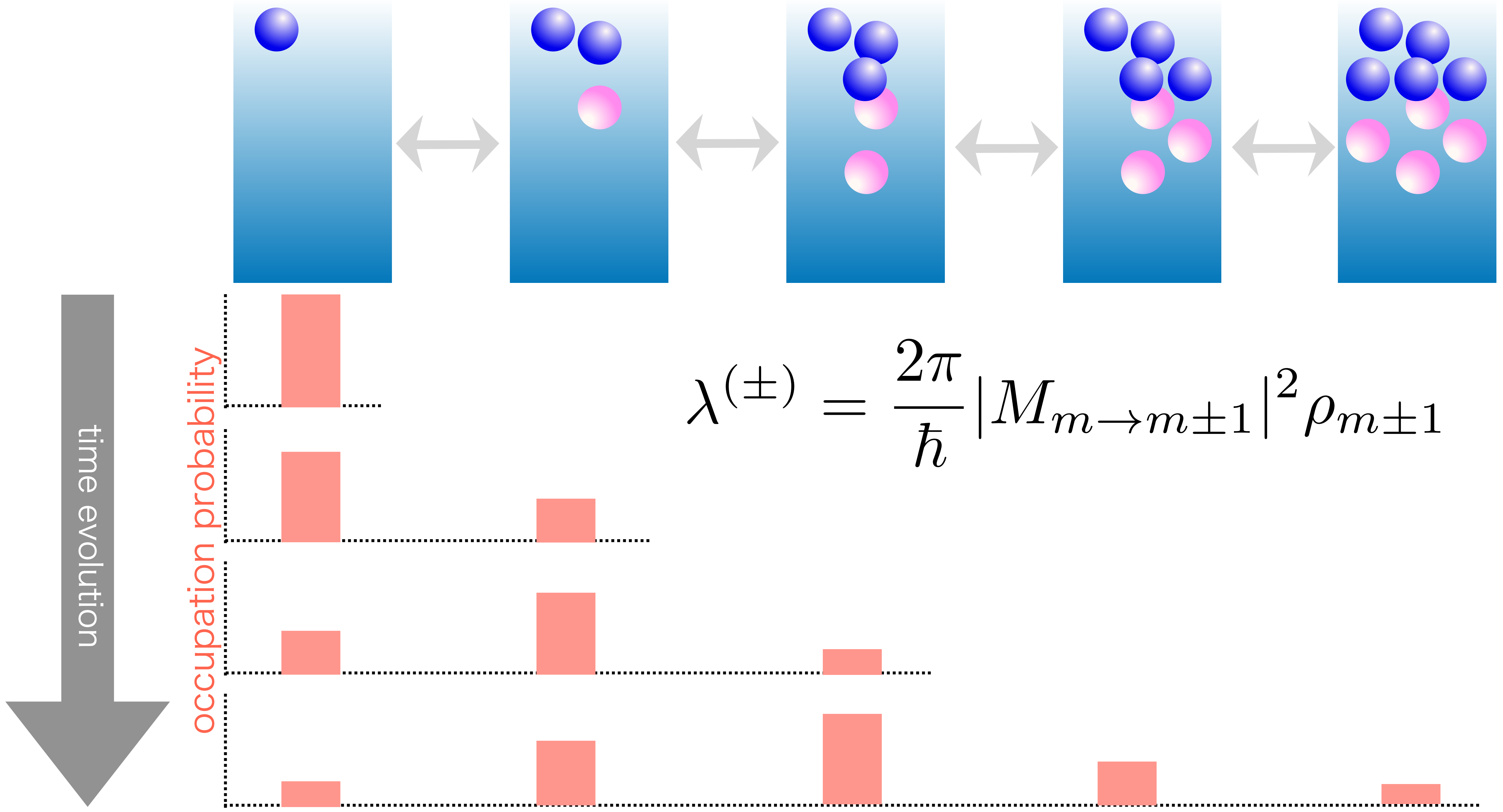
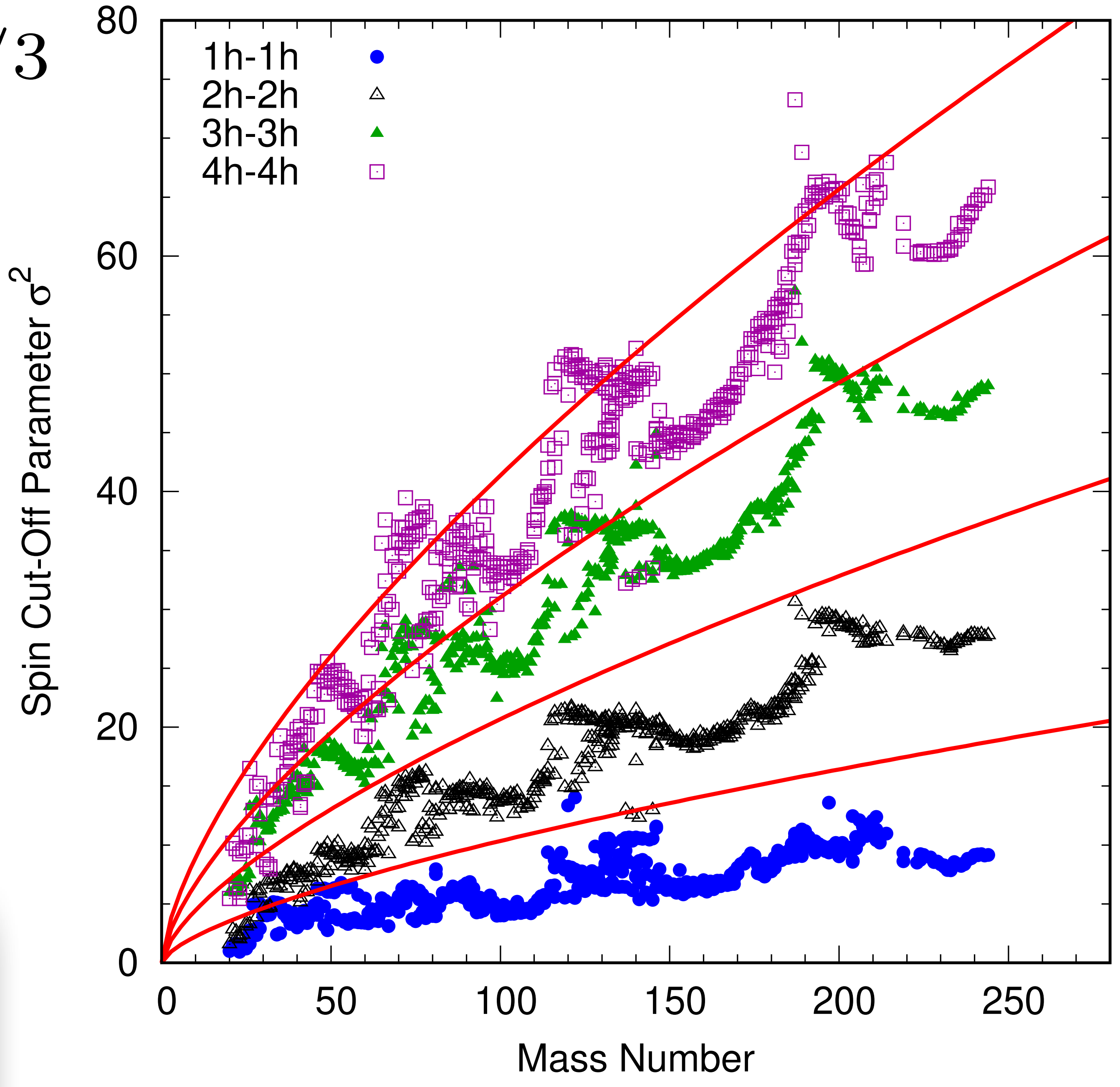
Time-Dependent Approach in Exciton Model - Master Equation



$$\lambda^{(\pm)} = \frac{2\pi}{\hbar} |M_{m \to m\pm1}|^2 \rho_{m\pm1}$$

- **Exciton model often creates more particle-hole states**
  - contrasts with the MSD one-step picture
  - because of the phenomenological parameters employed?
  - or some inherent problems in exciton?

$$\sigma^2 = 0.24nA^{2/3}$$



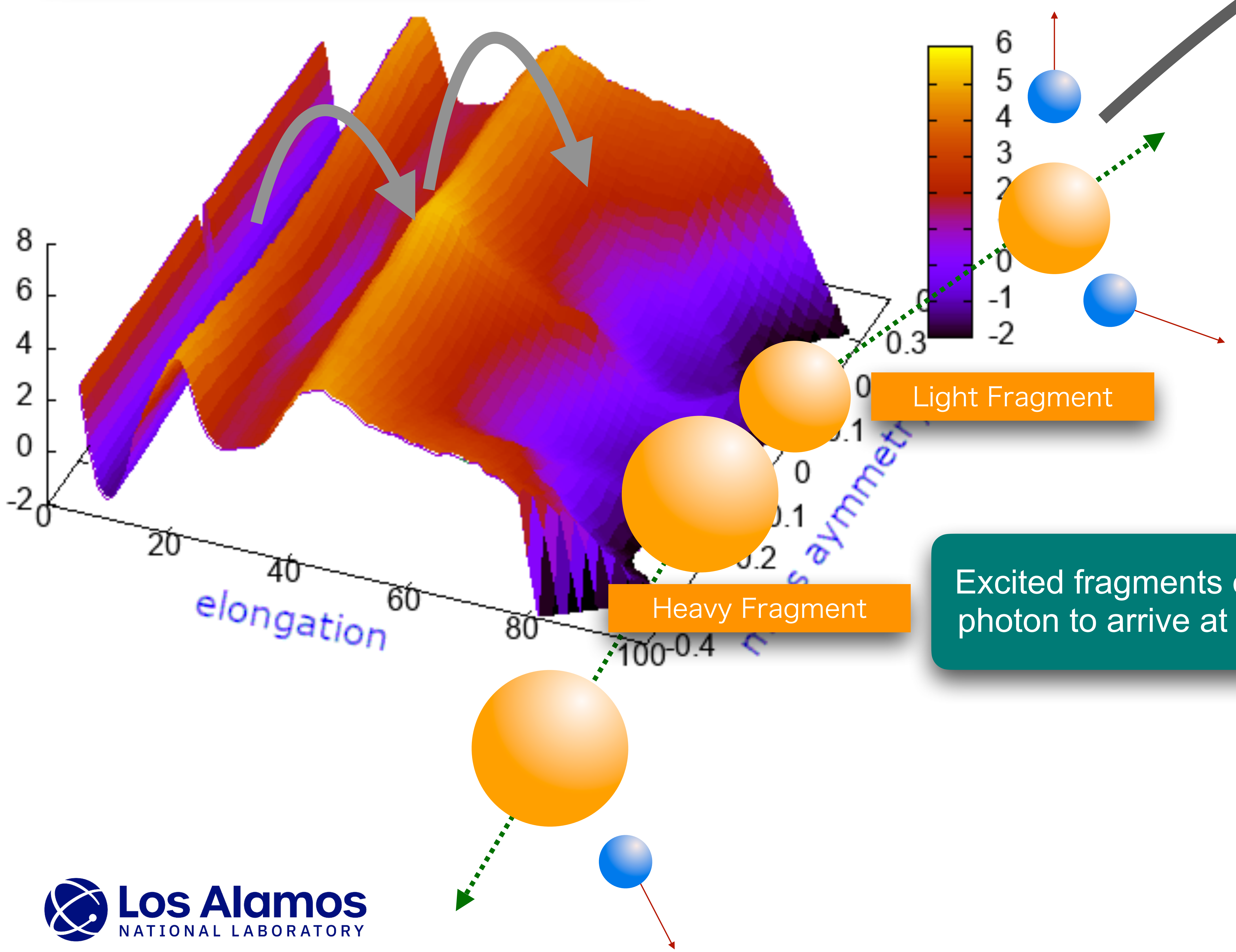
H. Sasaki, PRC112, 054607 (2025)

Because higher steps are implicitly included in Exciton, we needed a smaller values than 0.24

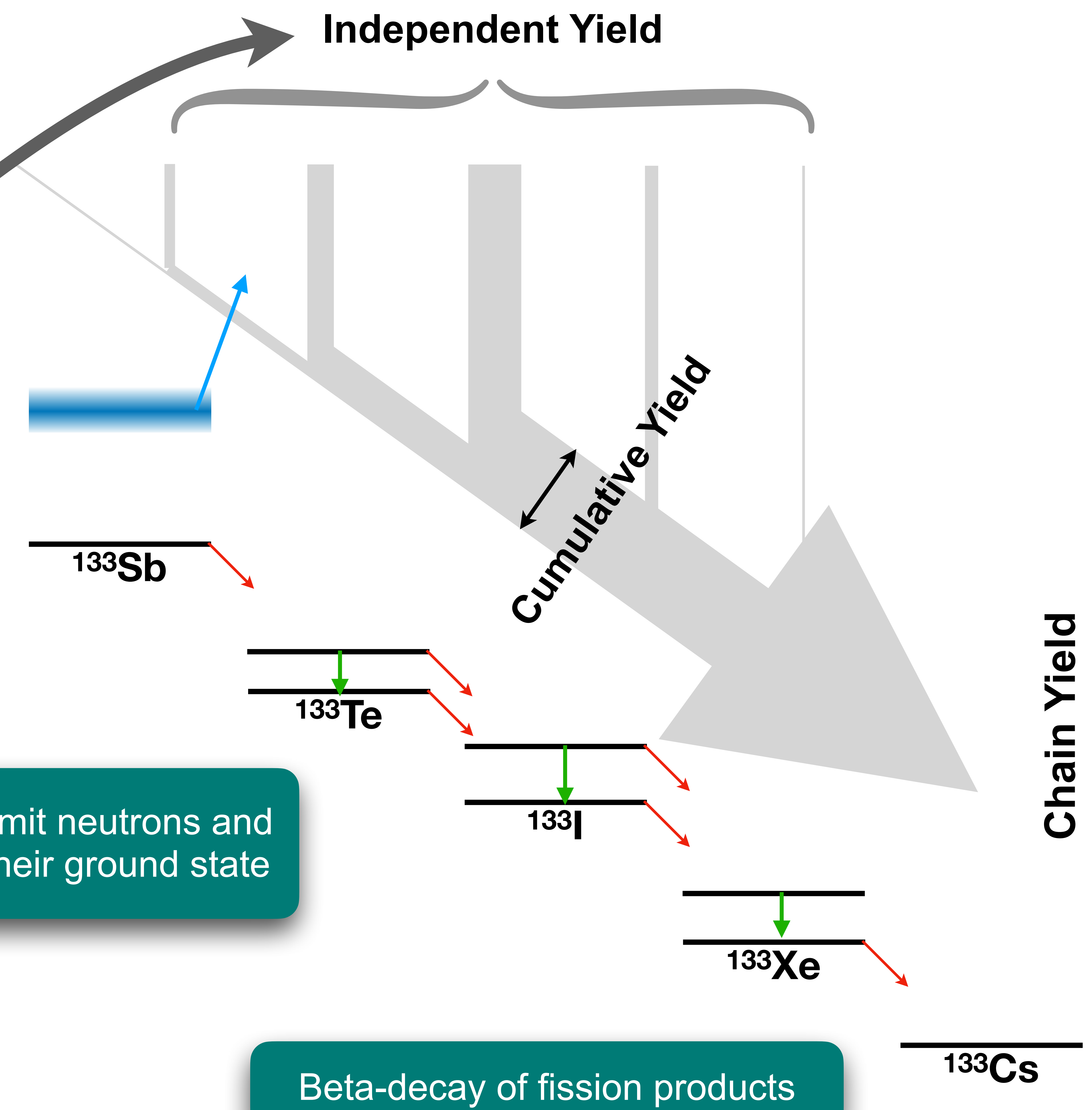
We need a new exciton model that is more consistent with quantum mechanical pictures

Nuclear Structure and Reaction for Pre and Post Scission Phenomena

Dynamical process toward scission



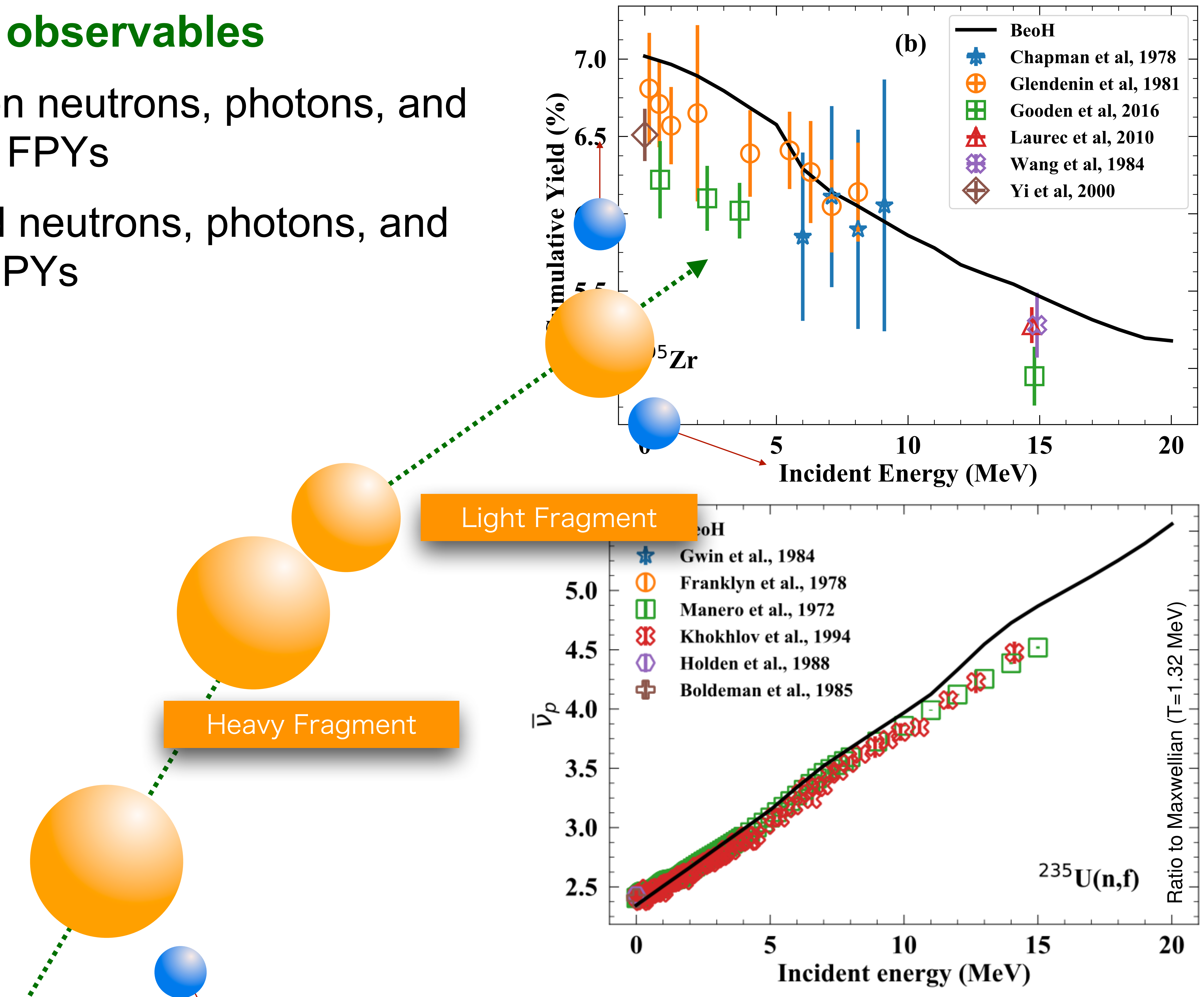
Excited fragments emit neutrons and photon to arrive at their ground state



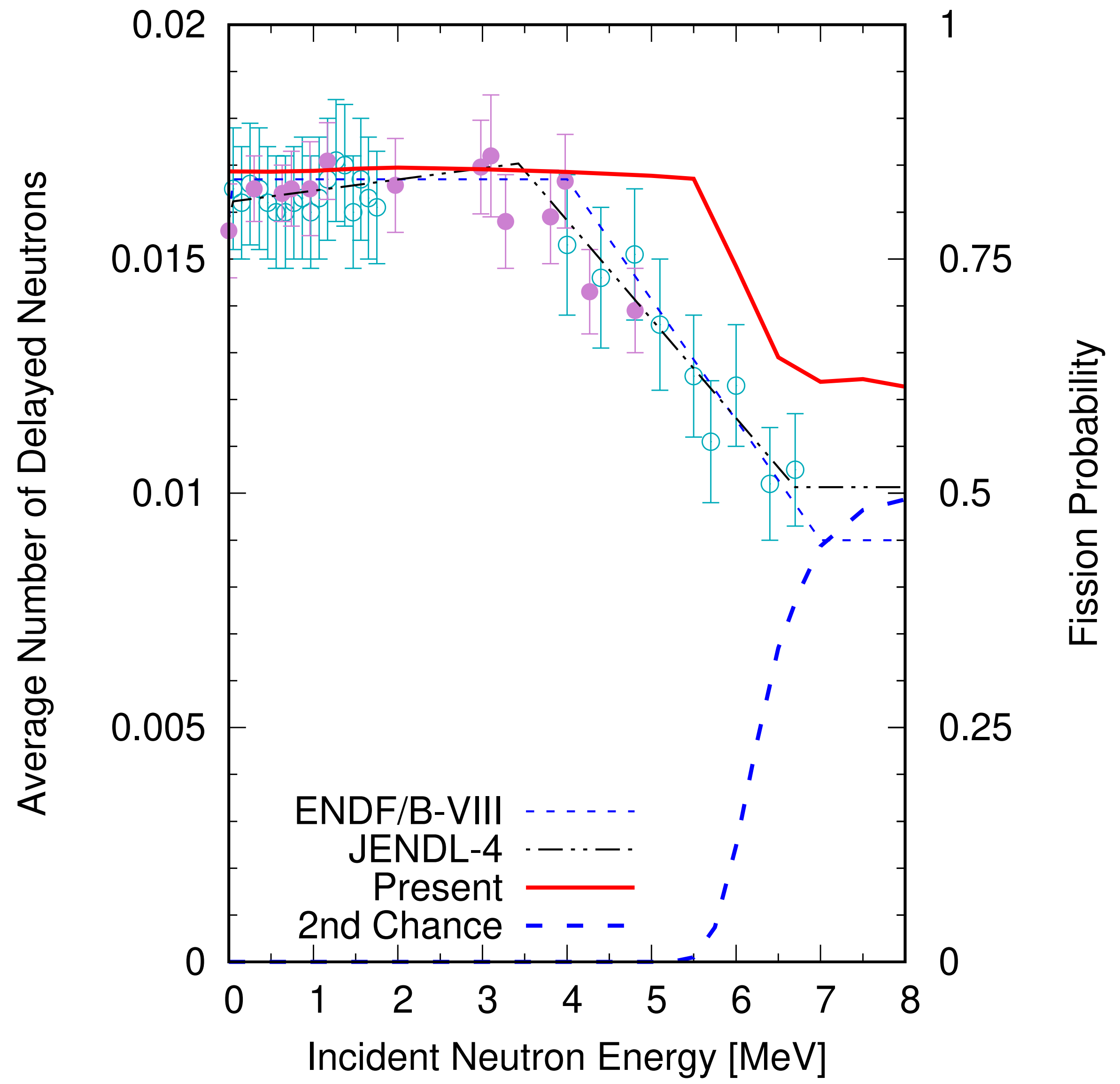
Beta-decay of fission products

Consistent Production of Various Fission Nuclear Data

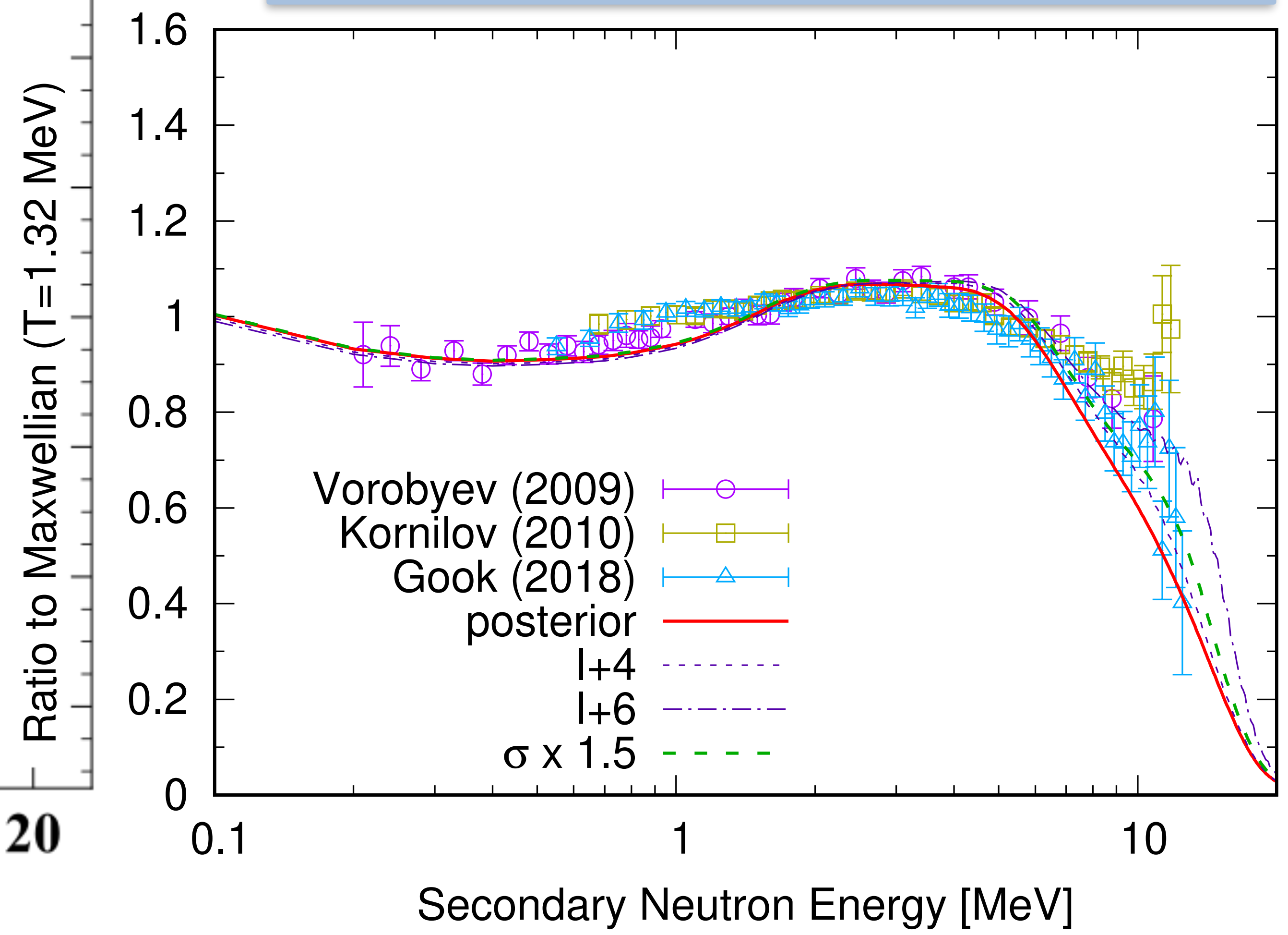
- **Post-scission observables**
  - prompt fission neutrons, photons, and independent FPYs
  - beta-delayed neutrons, photons, and cumulative FPYs



Lovell, PRC 103, 014615 (2021)

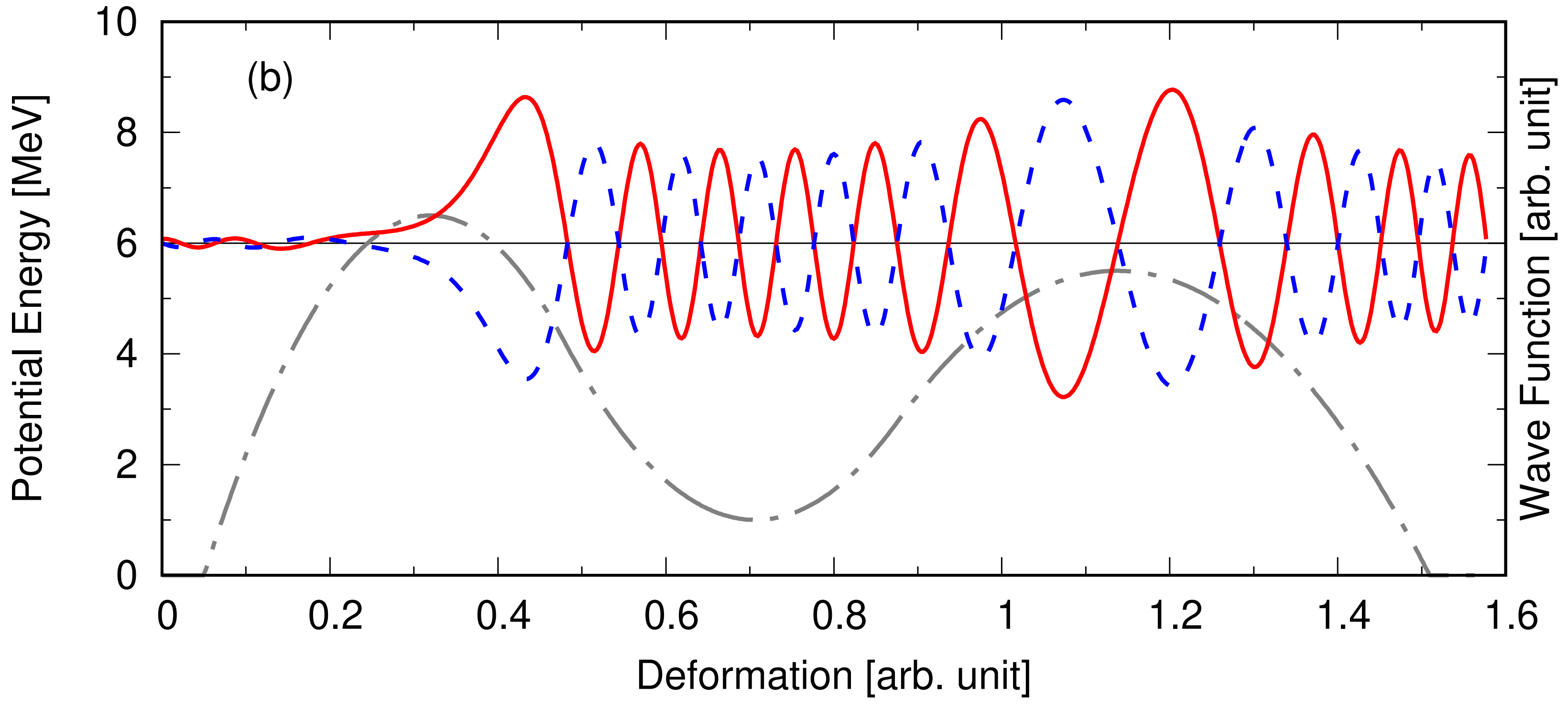


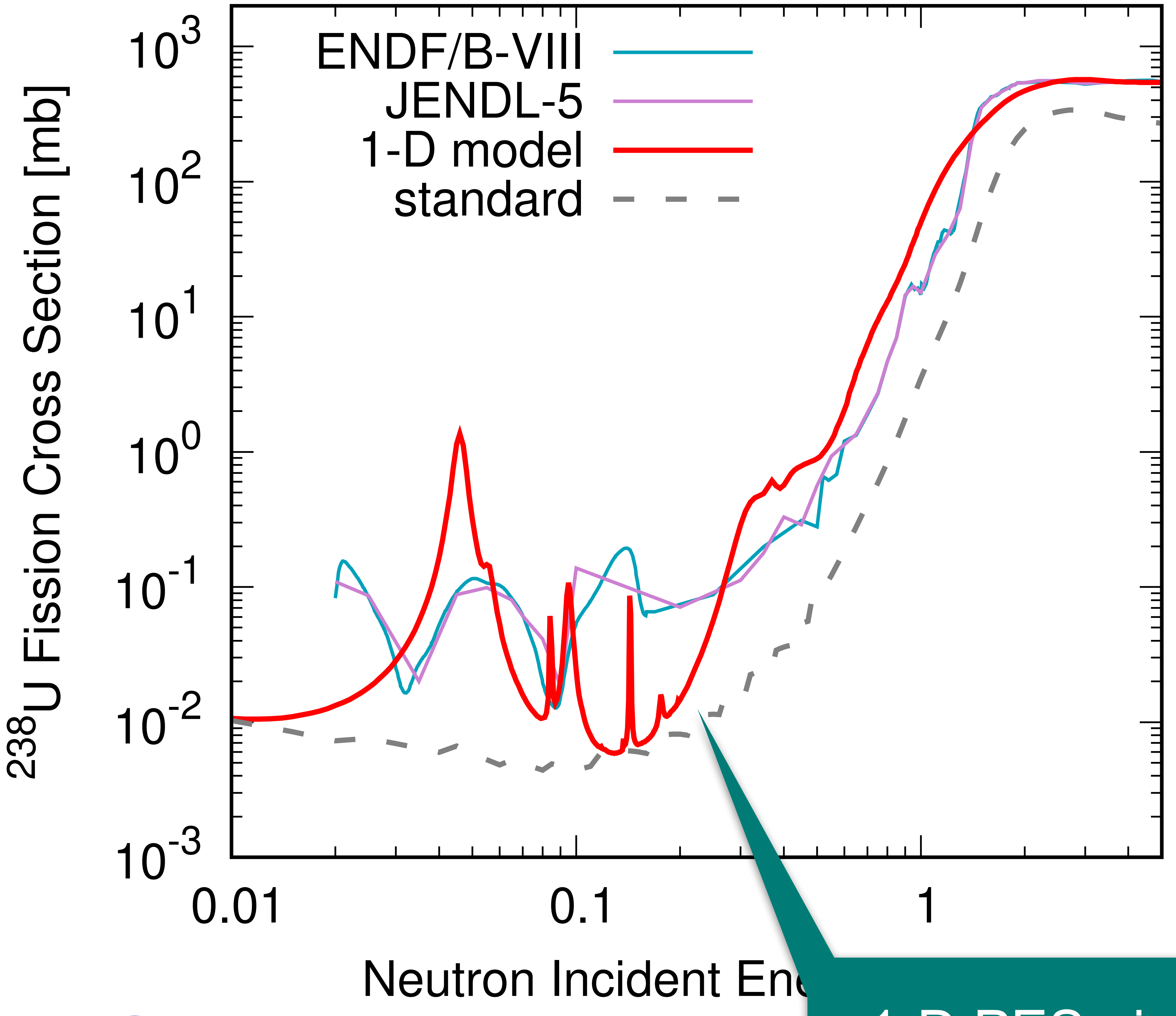
Okumura, JNST 59, 96 (2022)



Kawano, PRC104, 014611 (2021)

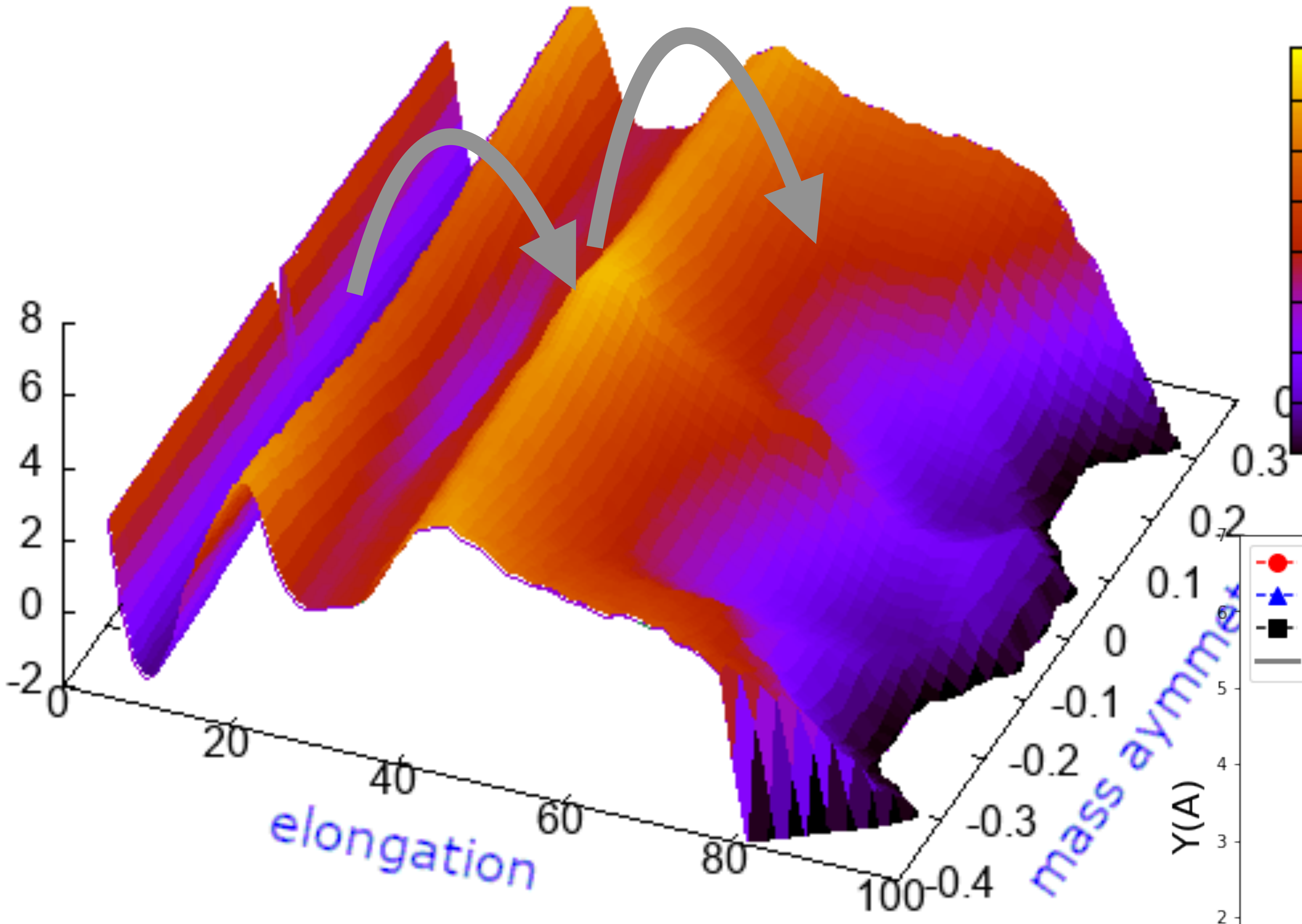
Connecting Pre- and Post Scission Phenomena

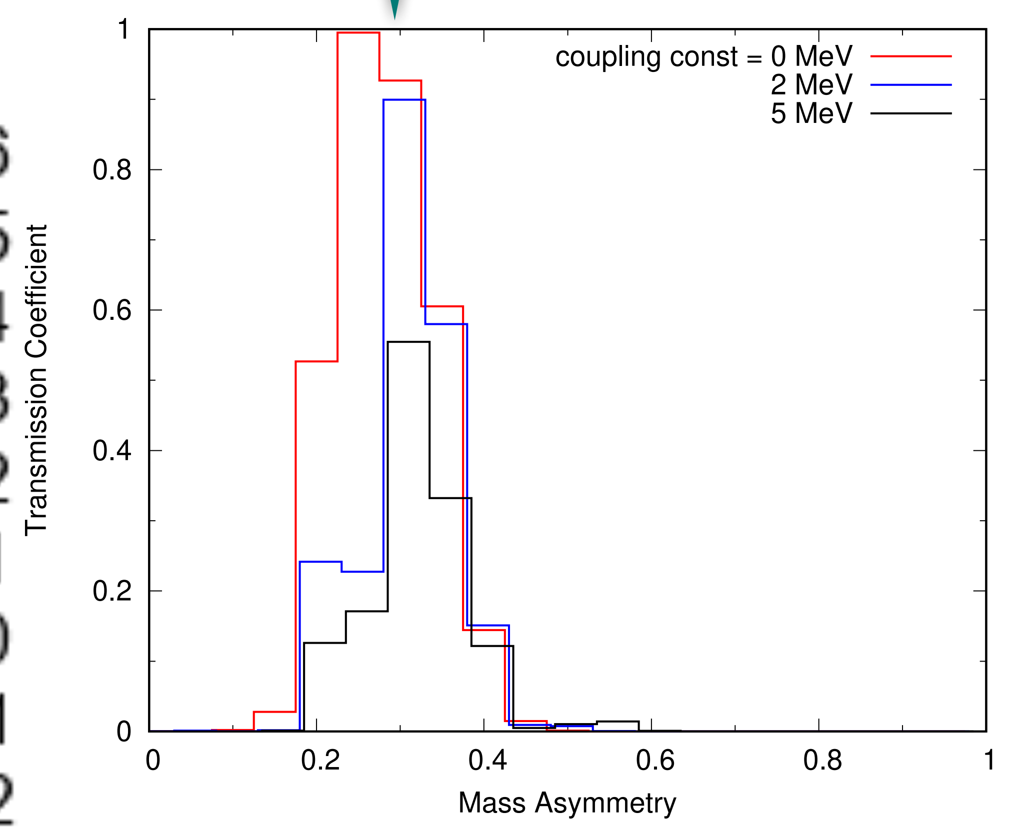


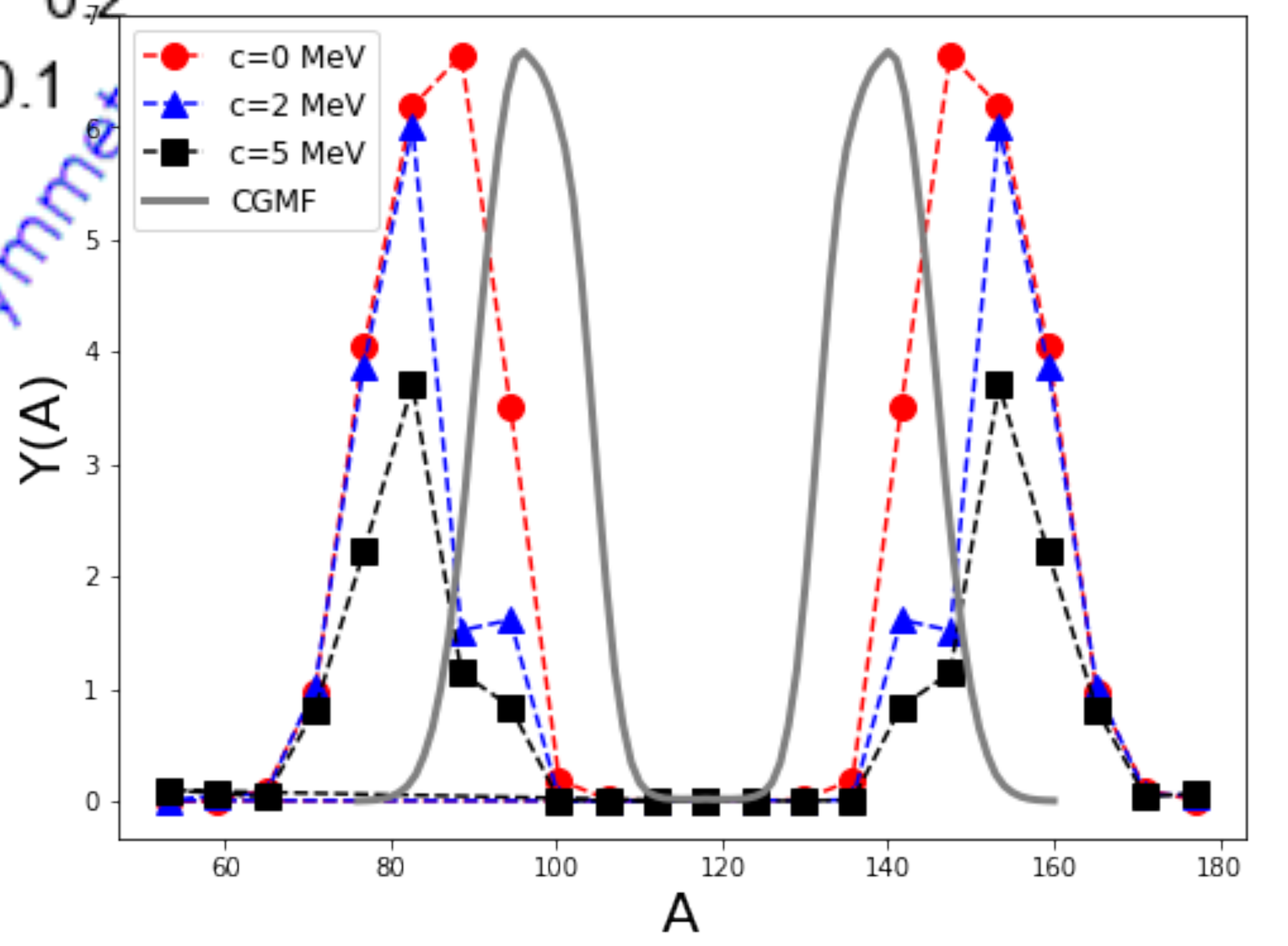


- **The final pieces to be unified**
  - PES, cross section, and FPY
  - 2-D solver under development

2-D PES gives both fission transmission and fragment yield



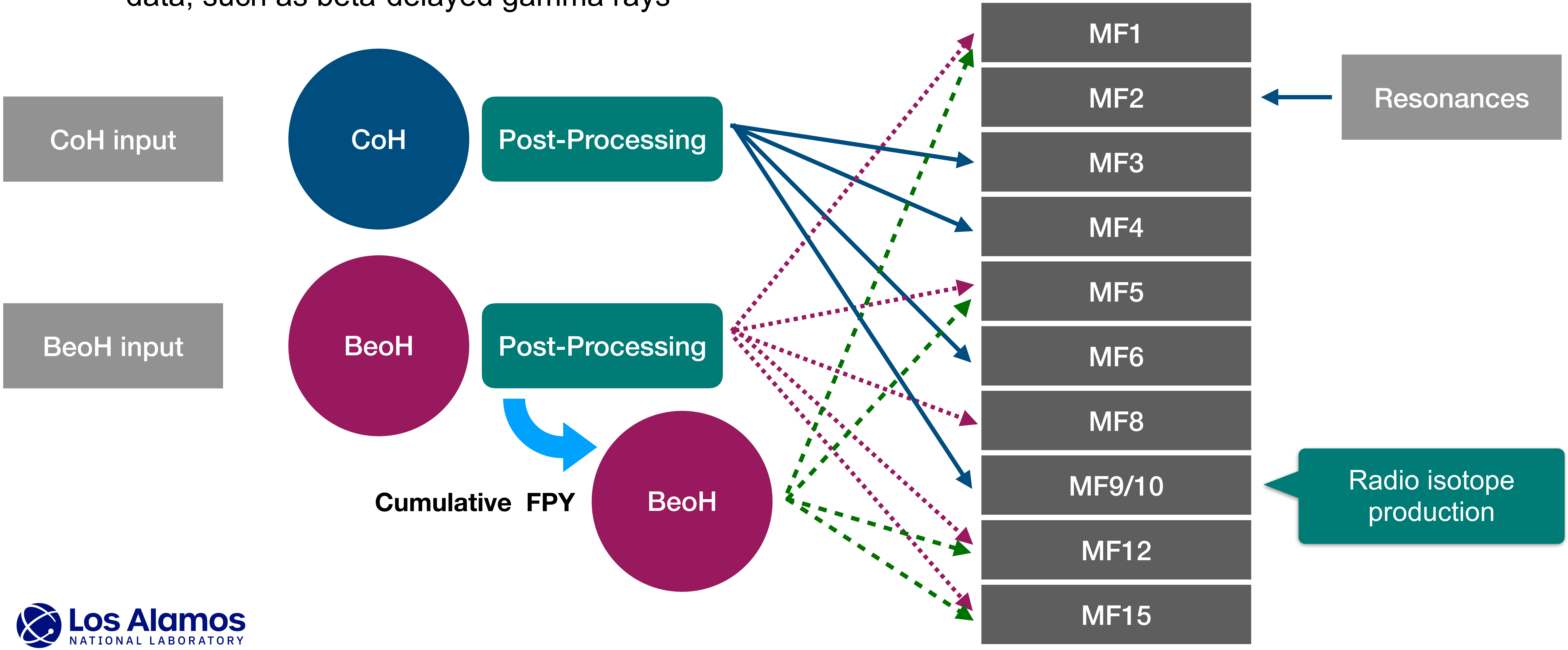




1-D PES gives fission transmission

Los Alamos CoH_3-based Evaluation: LACE

- **Production of all nuclear data using the CoH_3 and BeoH codes (with external resonance files)**
  - Facilitate to produce evaluated nuclear data files automatically, and provide not-so-commonly used data, such as beta-delayed gamma rays



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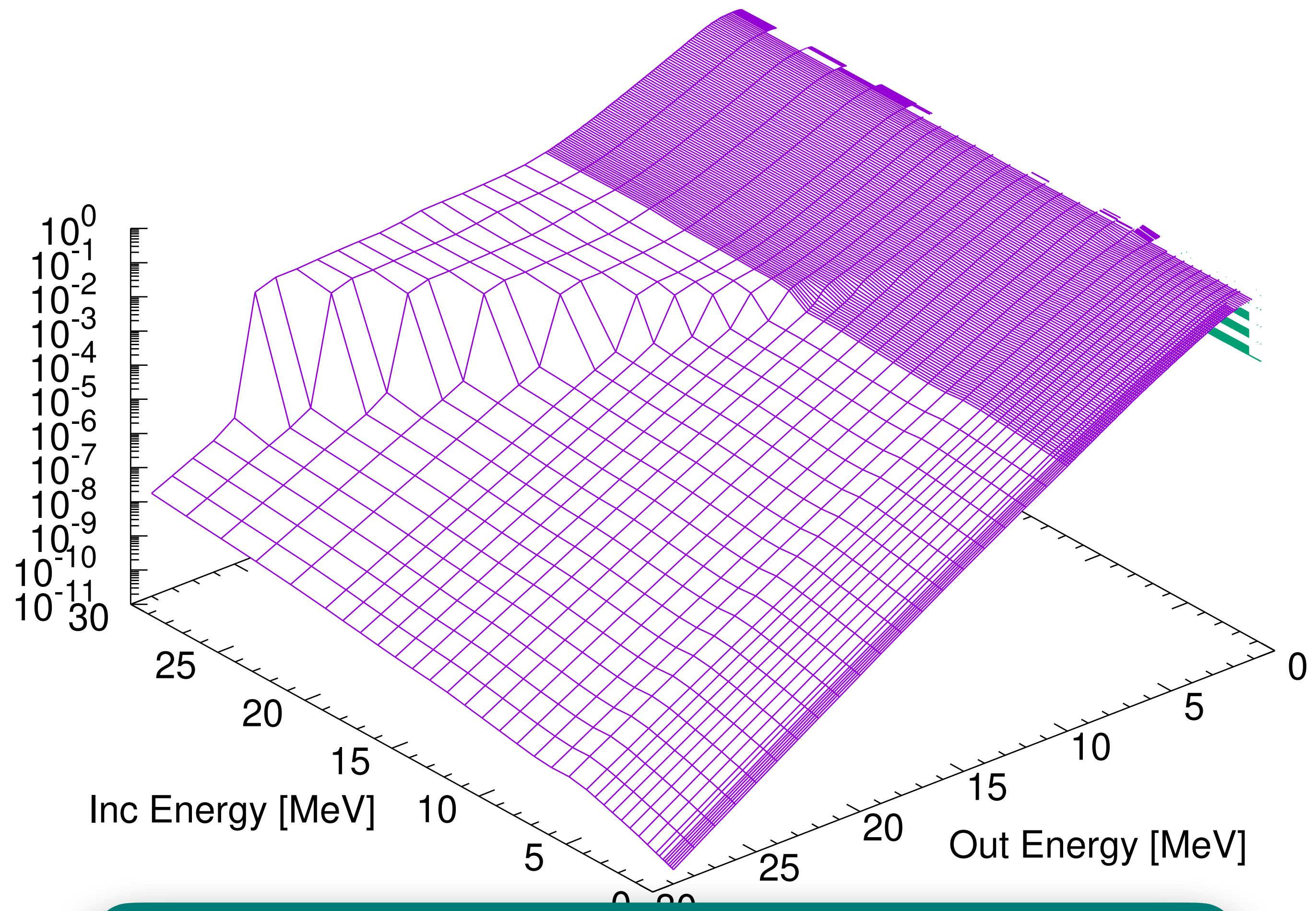
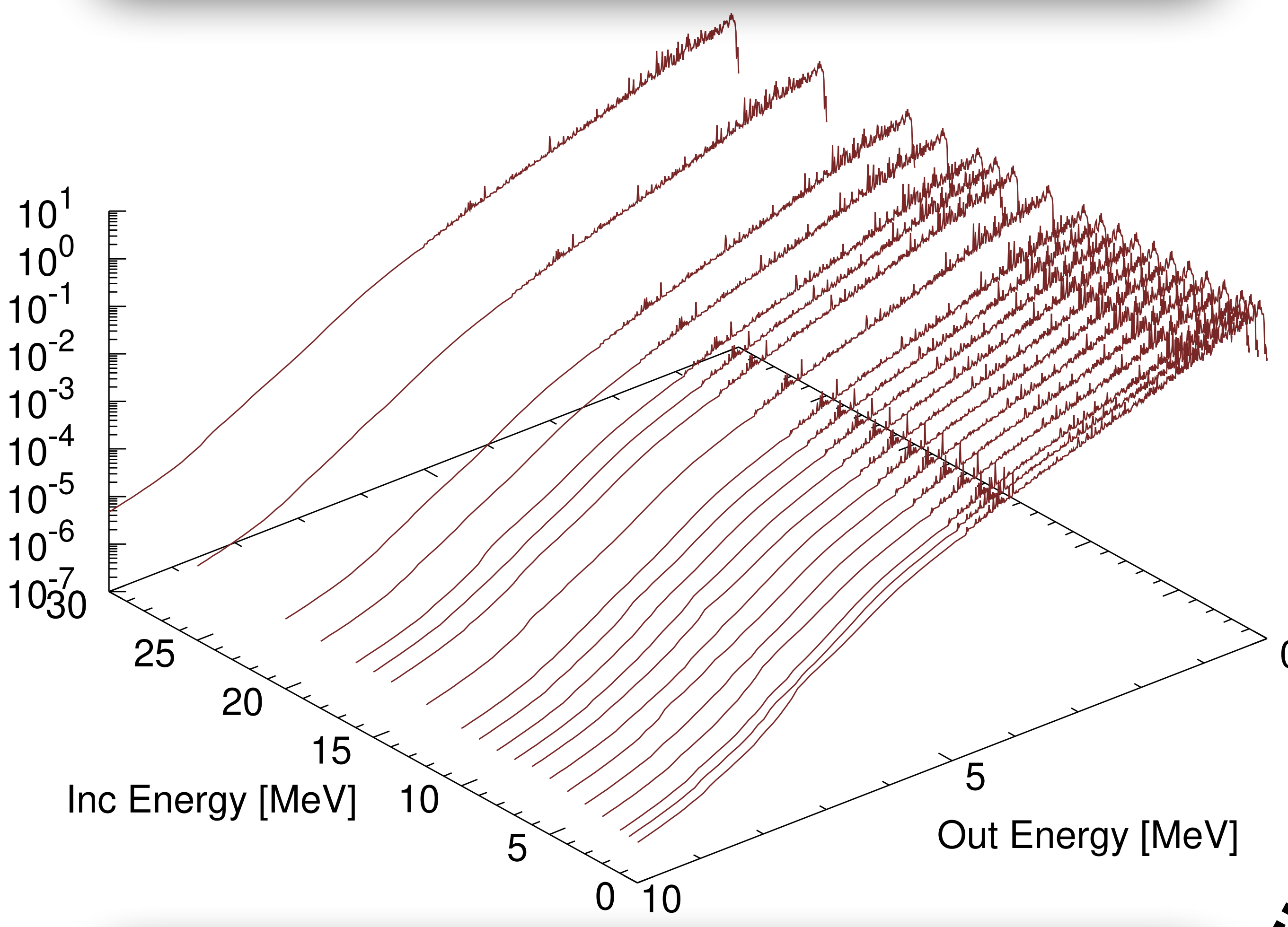
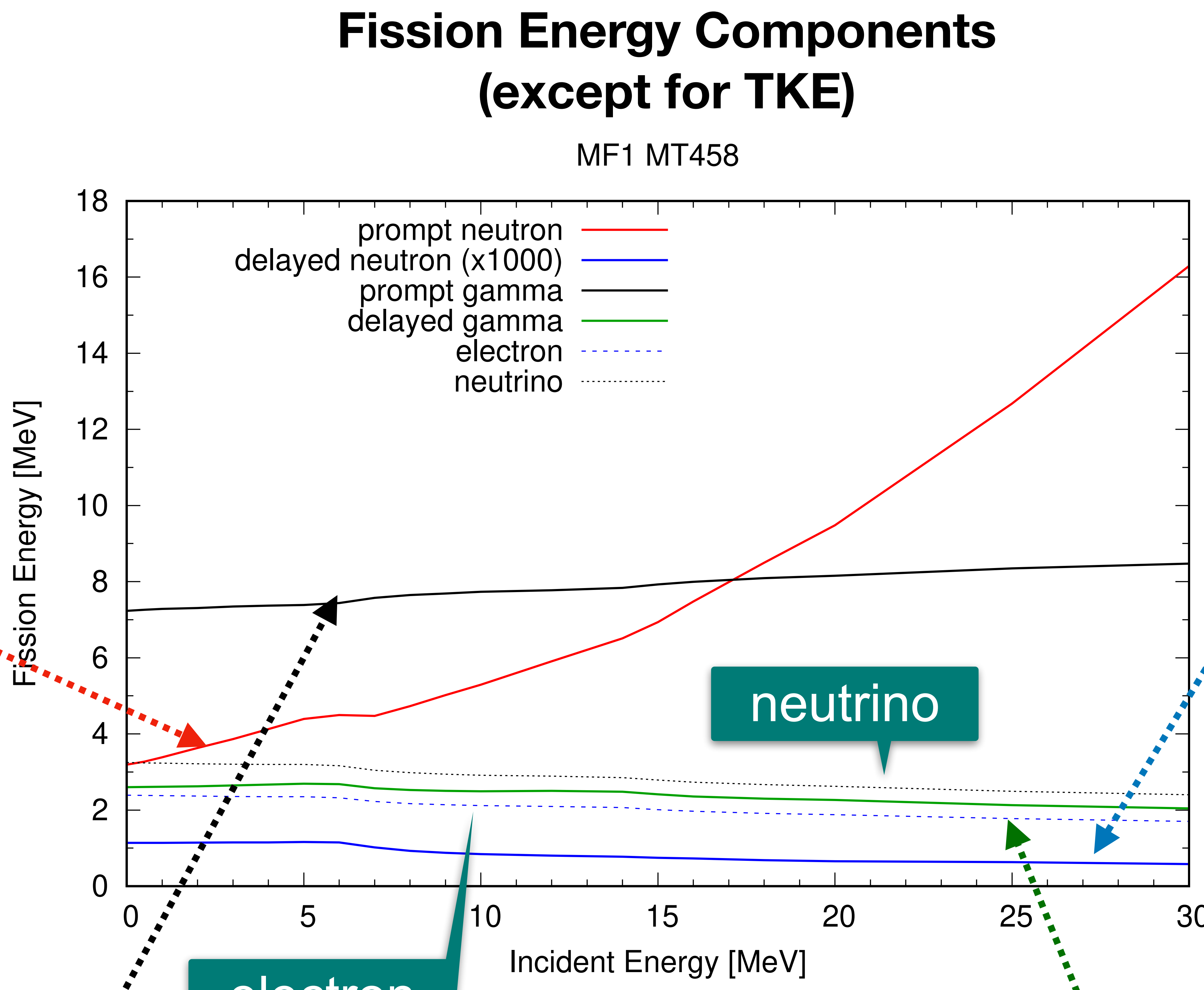
LACE Example ^{233}U Data



prompt neutron spectrum



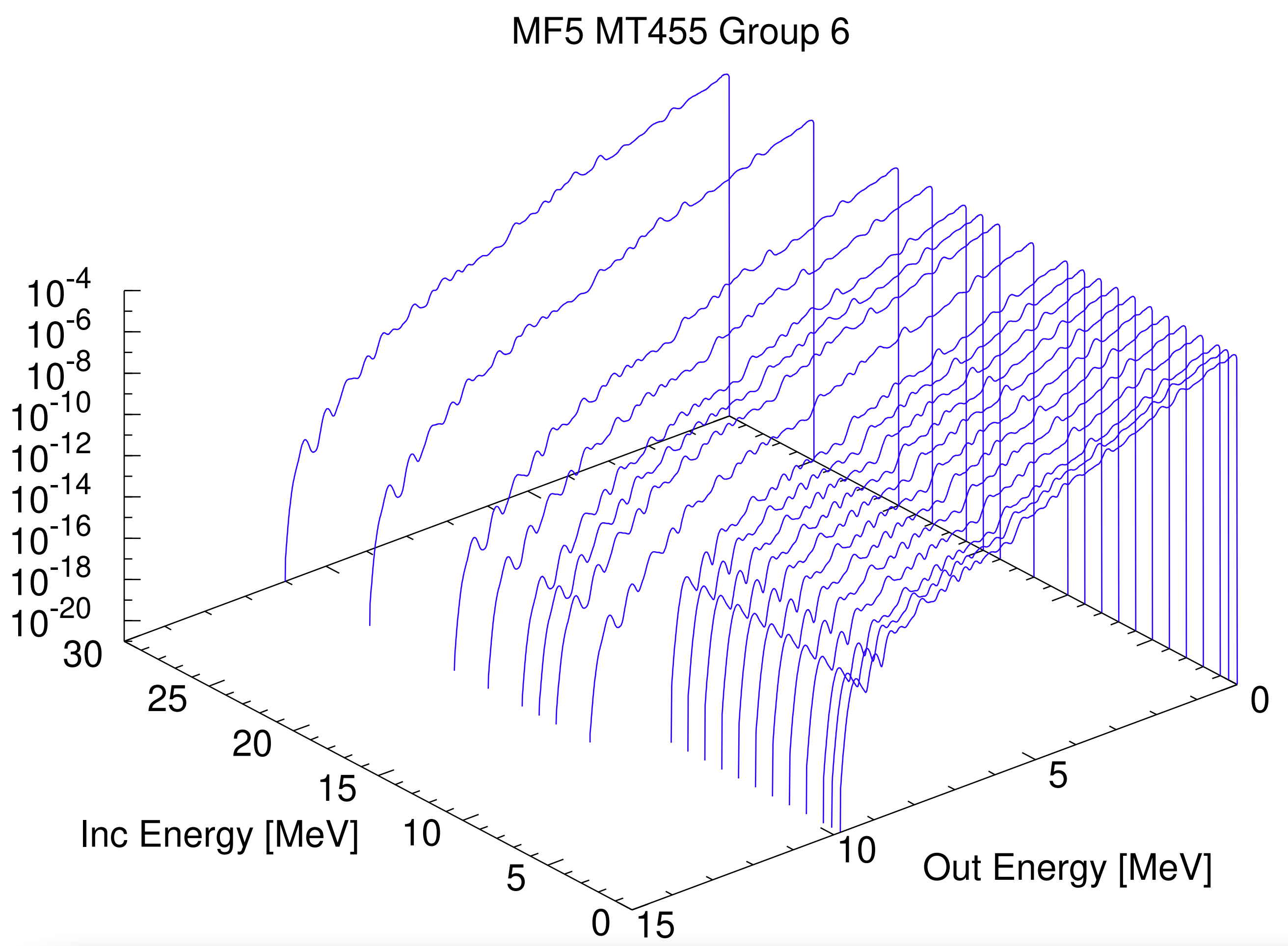
prompt gamma spectrum



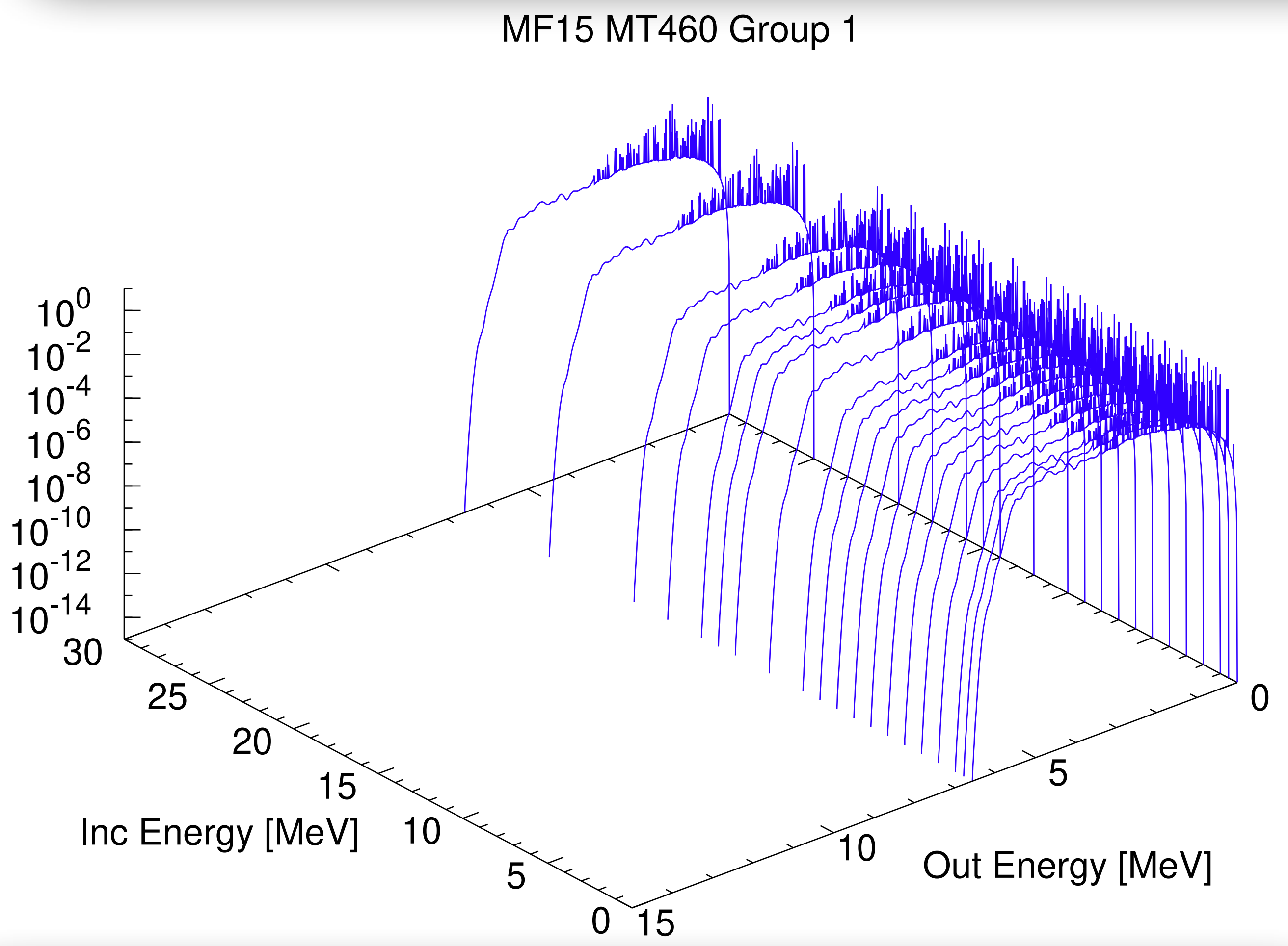
neutrino

electron

Production of complete nuclear data for actinides will be possible



delayed neutron (grp 6) spectrum



delayed gamma (grp 1) spectrum

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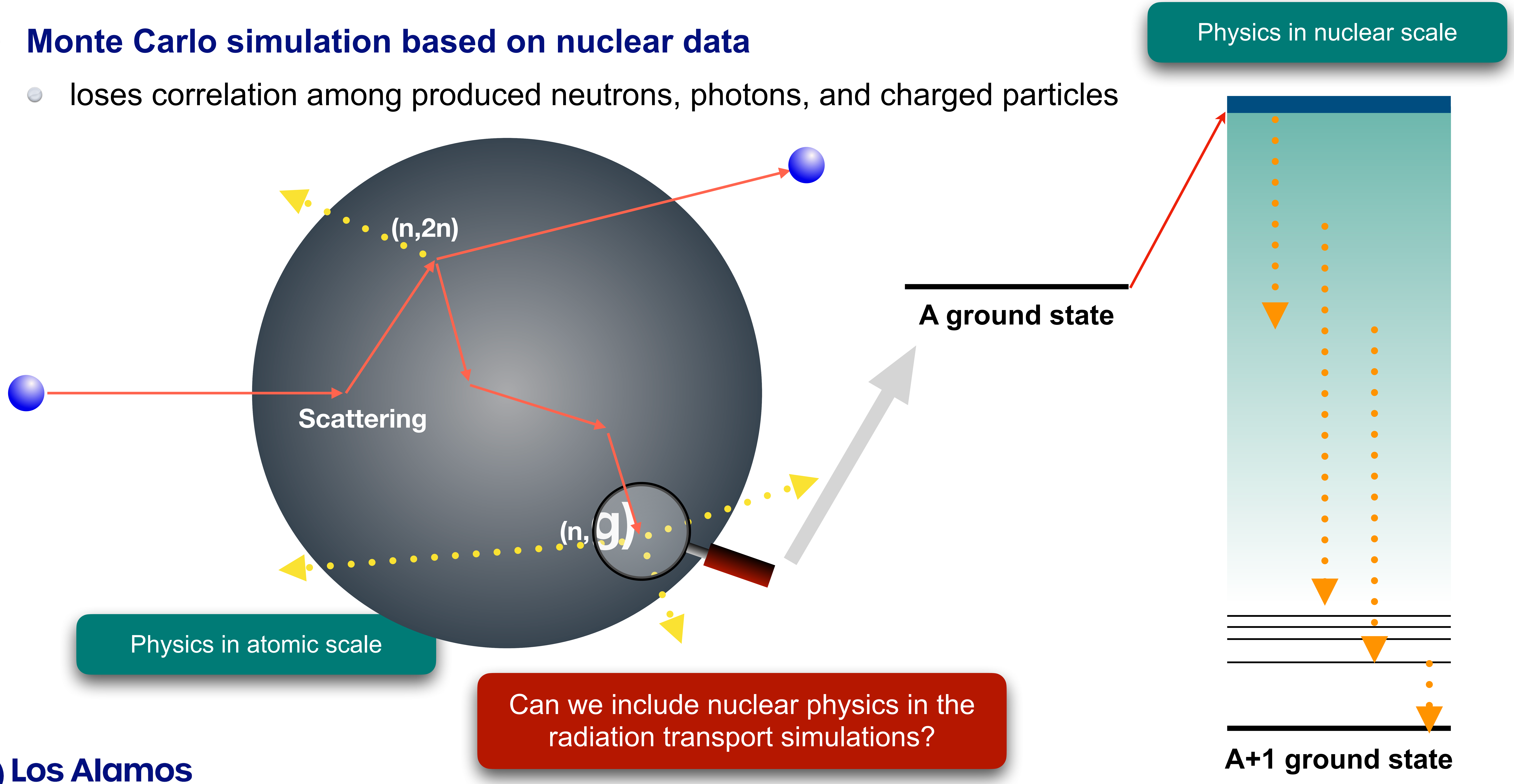
Multi-Scale Physics Radiation Transport Simulation

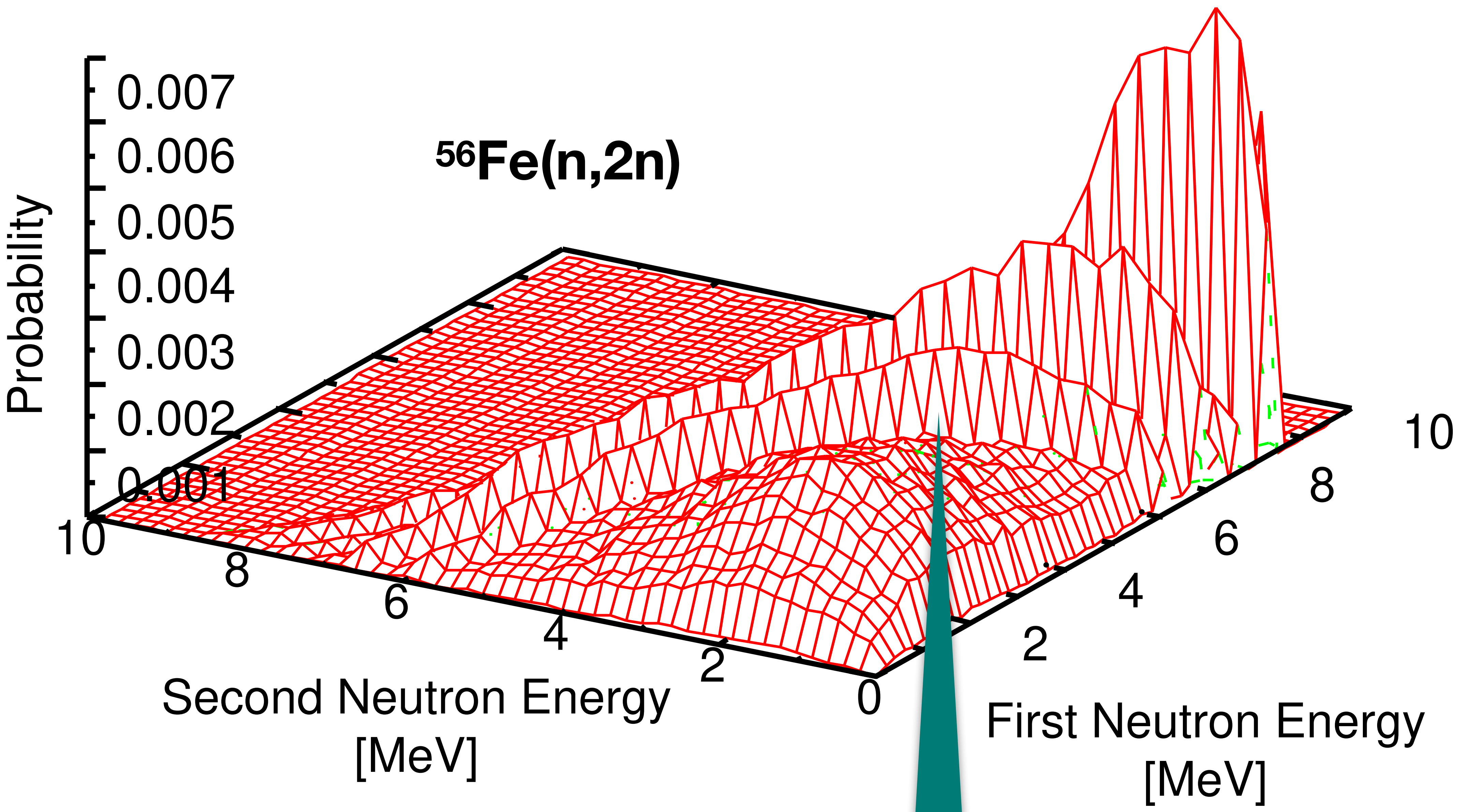
- **Monte Carlo simulation based on nuclear data**
  - loses correlation among produced neutrons, photons, and charged particles



Can we include nuclear physics in the radiation transport simulations?

Hauser-Feshbach Event Generator for Monte Carlo Transport

- **Event generators in MCNP**
  - CGMF (Hauser-Feshbach) and FREYA (evaporation) produce fission events
    - prompt neutrons and photons only



Because of pre-equilibrium, the first neutron tends to have higher energies

Kawano, JNST, 47, 462 (2010)

- **MC Hauser-Feshbach gives**
  - fully correlated particle productions
  - energy, spin, parity conservation at each event
- **MCHF codes already exist**
  - CoH_3 (LANL), YAHFC (LLNL)
- **Many applications we envisage**
  - detector response
  - semiconductor failures
  - active interrogation, etc

Since computers have been significantly advanced, HF event generator could be feasible in the next decade

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Concluding Remarks

- **Notable improvements in nuclear theories relevant to nuclear data reviewed**
  - capture, fission, inelastic scattering significantly improved in the last decade
  - more quantum mechanical approaches have been involved
    - QRPA/FAM for direct and pre-equilibrium processes demonstrated a breakthrough
- **Deficiencies in our current modeling revealed**
  - QM approach and exciton model for the pre-equilibrium process are incompatible
  - further works need to reconcile these two approaches
- **Maintaining model codes essential to implement of advanced nuclear theories**
  - automatic production of complete nuclear data files became (or almost becomes) possible
  - make them open-source to stimulate nuclear science communities
- **Extinction of nuclear data files**
  - beyond the traditional radiation transport simulations, the event generator could make great strides in applications of nuclear reaction physics